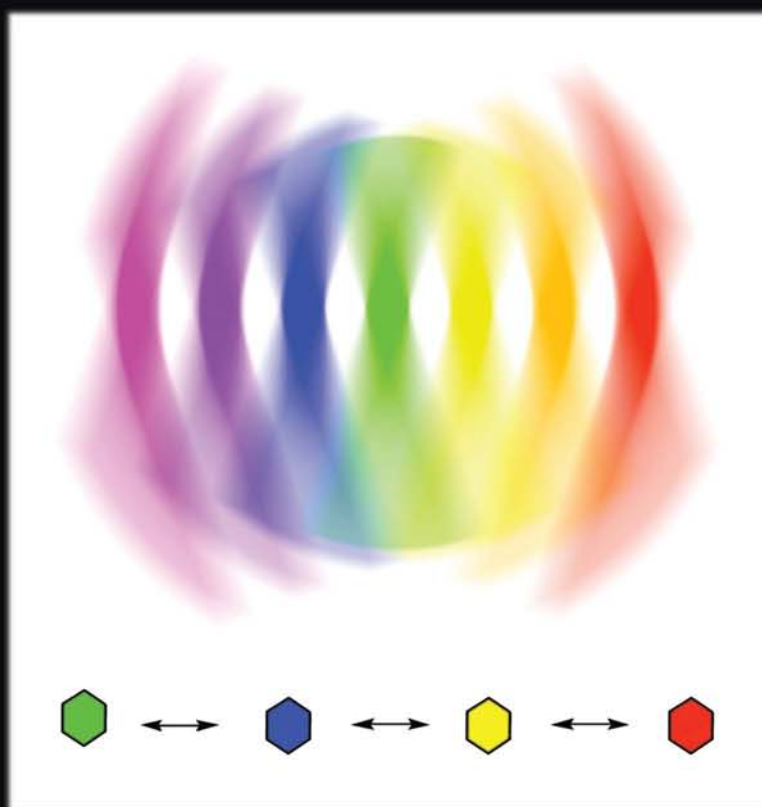


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HANDBOOK OF ACID-BASE INDICATORS

R. W. SABNIS



HANDBOOK OF
ACID-BASE
INDICATORS

HANDBOOK OF ACID-BASE INDICATORS

R. W. SABNIS

Squire, Sanders & Dempsey LLP
San Francisco, U.S.A.



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Dedication

to

My Guru/Mentor/Advisor

Prof. D. W. Rangnekar

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Preface

Color change has been a fascination of individuals for a long time. The two major types of dyes which are traditionally used for color change are leuco dyes and acid–base indicators. Leuco dyes are of limited use because three components are required to effect the color change transition. Generally, a color former (the leuco dye), a developer (such as phenolic compound) and a reversible matrix (such as a long chain alcohol) are combined. An often noted drawback with leuco dye systems is their water insolubility, thus, leuco dyes can only be used in solvent-based systems. Very few leuco dyes are commercially available. The synthetic methods of leuco dyes are complex, involve multiple steps, and do not generate high yields.

Acid–base indicators are also commonly known as pH indicators. Acid–base indicators are substances (dyes) which change color with pH. They are usually weak acids or bases, which when dissolved in water dissociate slightly and form ions. The major benefits of acid–base indicators over leuco dyes include: (a) acid–base indicators are one-component systems compared to three components required for a color change in leuco dye system; (b) acid–base indicators are generally soluble in organic solvent; they can be dissolved in water by making sodium or potassium salts and thus can be used in aqueous as well as solvent based systems; (c) acid–base indicators are commercially available or can be synthesized in excellent yield and purity.

There is no book available in the market directly on acid–base indicators even though use of acid–base indicators is widespread, growing rapidly and has exploded in the past two decades. There was a need to publish a book that provided an immediate incentive for compiling the notes to update the scientific community with the wealth of information on acid–base indicators. The literature in dyestuff chemistry, particularly on acid–base indicators, is largely in patents. This book provides a systematic and up-to-date library of information on 200+ acid–base indicators as a reference handbook. It was compiled as a resource guide for chemists and non-chemists in industry and university.

Acid–base indicators are arranged alphabetically by the most commonly used name. Again, the choice of primary name is somewhat arbitrary, but an effort has been made to strike a balance between names that are easily recognizable and names that are chemically informative. The detailed information of each acid–base indicator is covered in the following order: common name, other names, CA index name, CAS registry number, Merck index number (Merck Index 14th Edition, 2006), chemical structure, chemical/dye class, molecular formula, molecular weight, pH range, color change at pH, pKa, physical form, solubility, UV-visible (λ_{max}), melting point, boiling point, synthesis, major applications, safety/toxicity, and references of 200+ acid–base indicators. Where there are discrepancies between different values, the author used his judgment on selecting the most likely value.

Numerous recent references have been provided on various synthetic methods, major applications and safety/toxicity data. Space and format limitations prevent giving all the references for each indicator. This is the first book that provides safety/toxicity data with reference to acute toxicity, aquatic toxicity, carcinogenicity, cytotoxicity, ecotoxicity, genotoxicity, hemotoxicity, hepatotoxicity, mutagenicity, neurotoxicity, oral toxicity, phototoxicity, and phytotoxicity, and so forth.

Omissions as well as errors of fact and interpretation are inevitable in dealing with a vast subject such as acid–base indicators. I shall be glad to have my attention drawn to errors and to incorporate suggestions for improvement when a revision becomes possible.

I express my profound respect to my late-father, Wasudeo and late-mother, Suhasini who strained every resource to educate me. Words are inadequate to express my sincere appreciation to my wife

Madhuri and daughter Anika. It would not have been possible to write this book without their encouragement and patience. It is a great pleasure to express my gratitude and appreciation to CRC Press LLC (Taylor & Francis Group PLC) for giving me an opportunity to write this book.

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Ram W. Sabnis is currently a patent agent at Squire, Sanders & Dempsey L.L.P. in San Francisco, California, USA. His interests include dyes, pigments, organic chemistry, heterocycles, polymers, synthesis, formulations, coatings, displays, semiconductors, nanotechnology, biotechnology, medicinal chemistry, medical devices and patents. Presently, he focuses on writing and prosecuting U.S. and international patents, patentability opinions, and providing strong technical support. He is a registered patent agent with the U.S. Patent & Trademark Office (USPTO) and is also the inventor of more than 50 U.S. and international patents (issued/published). Prior to entering the legal (patents) field, he was a research chemist for Ascadia, General Electric, Brewer Science, U.S. Textiles and Invitrogen.



Dr Sabnis was born and raised in Mumbai, India. He received his M.Sc. in organic chemistry from University of Mumbai and Ph.D. in organic chemistry (Dyes) from University Institute of Chemical Technology (UICT), University of Mumbai, India. He is a fellow of the American Institute of Chemists, USA. He was awarded a chartered colourist and fellow of the Society of Dyers & Colourists, U.K.

Dr. Sabnis is one of the world's foremost experts in dyes, inventing the world's first colored bubbles (non-staining) and color changing dye system with many applications. He has more than 25 years of industrial and academic research experience in dye chemistry, particularly, dyes for biomedical (fluorescent probes), personal care products, health/beauty products, displays, inks, paints, plastics, textiles, and toys applications. He has written over 150 publications which include books, book chapters, patents, reviews, papers, and symposia presentations. Dr. Sabnis is a recipient of the Perkin Innovation Award by Society of Dyers & Colourist, U.K.; Grand Innovation Award by Popular Science, U.S.; Six Sigma Green Belt & Competitive Spirit Award by GE, U.S.; Best Doctoral Thesis Award by University of Mumbai, India. He will continue to focus his activities on fascinating dye chemistry as well as demanding intellectual property in the years to come.

A

A

ACID ALIZARIN VIOLET N

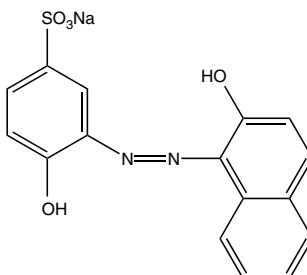
Other Names C.I. Mordant Violet 5; C.I. Mordant Violet 5, monosodium salt; Eriochrome Violet B; Acid Alizarin Violet N; Acid Alizarine Violet; Acid Alizarine Violet B; Acid Chrome Violet K; Acid Chrome Violet N; Aizen Chrome Violet BH; Alizarine Violet N; Alphacroic Violet B; Atlantichrome Violet B; Brasilan Chrome Violet B; C.I. 15670; Chromacid Violet R; Chromaven Violet B; Chrome Fast Violet B; Chrome Violet B; Chrome Violet K; Chrome Violet R; Cromal Violet B; Diacromo Violet N; Diamond Corinth N; Durochrome Violet B; Erio Chrome Violet BA; Erio Chrome Violet BR; Hispacrom Violet B; Java Chrome Violet B; Magracrom Violet N; Mitsui Chrome Violet BC; Monochrome Violet B; Mordant Violet 5; Omega Chrome Dark Violet D; Pontachrome Violet SW; Solochrome Violet; Solochrome Violet R; Solochrome Violet RS; Solocrom Violet RS; Sunchromine Violet B; Superchrome Violet B; Symulon Chrome Violet B; Tetrochrome Violet N; Yodochrome Violet B

CA Index Name Benzenesulfonic acid, 4-hydroxy-3-[(2-hydroxy-1-naphthalenyl)azo]-, monosodium salt

CAS Registry Number 2092-55-9

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula $C_{16}H_{11}N_2O_5SNa$

Molecular Weight 366.33

pH Range 6.5–9.0

Color Change at pH Orange-red (6.5) to violet (9.0)

pKa 4.35, 7.4, 9.35

Physical Form Reddish-violet crystals

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 501 nm

Melting Point >300°C

Synthesis Synthetic methods¹⁻³

Major Applications inks,⁴ dye lasers,⁵ in manufacture of vinyl polymers,⁶ textiles¹ determination of iron,⁷ calcium,⁸ aluminum,⁹⁻¹¹ tantalum,¹² monitoring hardness in industrial water,¹³ measuring chlorine dioxide in drinking water,¹⁴ hypoglycemic agents,¹⁵ nuclear fluorochrome¹⁶

Safety/Toxicity Mutagenicity¹⁷

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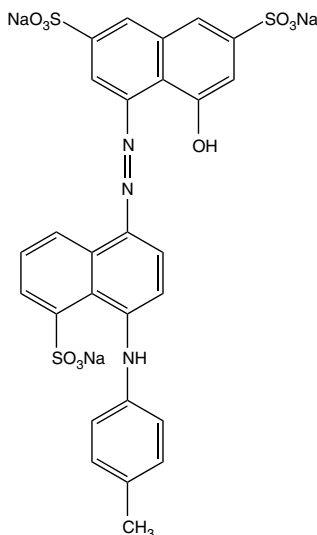
ACID BLUE 89

Other Names C.I. Acid Blue 89, trisodium salt; Acid Blue Sh; Acid Light Blue; Acid Sky Blue; Acilan Fast Navy Blue B; Atul Acid Sulfon Blue B; C.I. 13405; C.I. Acid Blue 89; Calcocid Wool Blue B; Cirene Brilliant Blue B; Eniacid Brilliant Blue B; Fast Wool Blue B; Hispacid Fast Blue B; Russian Acid Blue; Sulfonine Acid Blue B; Sulphon Acid Blue B; Tertracid Fast Flue SB

CA Index Name 2,7-Naphthalenedisulfonic acid, 4-hydroxy-5-[[4-[(4-methylphenyl)amino]-5-sulfo-1-naphthalenyl]azo]-, trisodium salt

CAS Registry Number 10359-95-2

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Azo

Molecular Formula C₂₇H₁₈N₃O₁₀S₃Na₃

Molecular Weight 709.61

pH Range 11.0–12.0

Color Change at pH Blue (11.0) to red (12.0)

pKa 11.29

Physical Form Brown powder

Solubility Soluble in water, ethanol

Melting Point >250°C

Synthesis Synthetic method¹

Major Applications Wool dyeing,² tints for polyester fibers,³ coloring metal oxide⁴

Safety/Toxicity No data available

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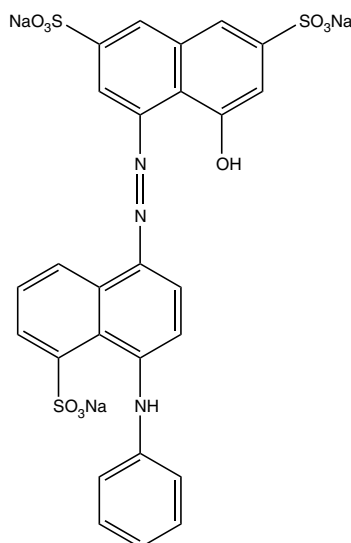
ACID BLUE 92

Other Names Acid Blue 2K; C.I. Acid Blue 92; C.I. Acid Blue 92, trisodium salt; 4-[(4-Anilino-5-sulfo-1-naphthyl)azo]-5-hydroxy-2,7-naphthalenedisulfonic acid trisodium salt; Acid Blue 92; Acid Blue A; Acid Fast Blue R; Acid Leather Blue R; Acid Wool Blue RL; Acilan Fast Navy Blue R; Airedale Blue RL; Amacid Fast Blue R; Anazolene sodium; Benzyl Blue R; Benzyl Fast Blue R; Best Acid Blue 3R; Bucacid Fast Wool Blue R; C.I. 13390; C.I. Solvent Blue 37; Calcocid Fast Blue SR; Caracid Cyanine Blue R Conc PDR; Cirene Brilliant Blue R; Colacid Blue A; Coomassie Blue Medicinal; Coomassie Blue RL; Cyanine Acid Blue R; Cyanine Acid Blue R New; Fast Acid Blue RL; Fast Wool Blue R; Fenazo Blue SR; Hispacid Fast Blue R; Kayanol Navy Blue R; Lampronol Blue BR; Luxol Fast Blue AR; Luxol Fast Blue ARN; Medium Blue EMBL; Methasol Blue RL; Methasol Blue RLX; Pontacyl Fast Blue R; Sepisol Fast Blue ARNF; Sodium anazolene; Solvent Blue 37; Sulfonine Acid Blue R; Sulphon Acid Blue R; Sulphon Acid Blue RA; Sulphon Acid Blue RA Extra; Suminol Fast Navy Blue R; Tertracid Fast Blue SR; Trisodium 4'-anilino-8-hydroxy-1,1'-azonaphthalene-3,6,5'-trisulfonate; Vondamol Fast Blue R; Wool Blue RL; Wool Fast Blue R

CA Index Name 2,7-Naphthalenedisulfonic acid, 4-hydroxy-5-[[4-(phenylamino)-5-sulfo-1-naphthalenyl]azo]-, trisodium salt

CAS Registry Number 3861-73-2

Merck Index Number 628

Chemical Structure

Chemical/Dye Class Azo

Molecular Formula $C_{26}H_{16}N_3O_{10}S_3Na_3$

Molecular Weight 695.59

pH Range 11.0–12.0

Color Change at pH Blue (11.0) to pink (12.0)

pKa 11.22

Physical Form Dark bluish-black powder

Solubility Soluble in water, acetone; slightly soluble in ethanol, glycerol

UV-Visible (λ_{max}) 571 nm, 585 nm, 580–590 nm

Melting Point >300°C

Synthesis Synthetic methods^{1–6}

Major Applications Color filter,^{7,8} fuel cells,⁹ thin films,¹ inks,¹⁰ markers,¹¹ lithographic printing plates,¹² textiles,¹³ cosmetics,¹⁴ neural network¹⁵

Safety/Toxicity Genotoxicity¹⁶

A

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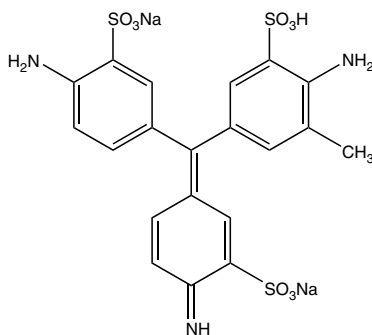
ACID FUCHSIN

Other Names C.I. Acid Violet 19; C.I. Acid Violet 19, disodium salt; Rubine S; Acid Fuchsin; Acid Fuchsin FB; Acid Fuchsin N; Acid Fuchsin O; Acid Fuchsin S; Acid Leather Magenta A; Acid Magenta; Acid Magenta O; Acid Violet 19; Acid fuchsin sodium salt; Acid rosein; Acid rubin; Acidal Fuchsin; Acidal Magenta; C.I. 42685; Fuchsin S; Fuchsin acid; Fuchsin acid; Kiton Magenta A; *p*-Fuchsin acid

CA Index Name Benzenesulfonic acid, 2-amino-5-[(4-amino-3-sulphophenyl)(4-imino-3-sulfo-2,5-cyclohexadien-1-ylidene)methyl]-3-methyl-, disodium salt

CAS Registry Number 3244-88-0

Merck Index Number 107

Chemical Structure

Chemical/Dye Class Triphenylmethane

Molecular Formula $C_{20}H_{17}N_3O_9S_3Na_2$

Molecular Weight 585.55

pH Range 12.0–14.0

Color Change at pH Red (12.0) to colorless (14.0)

Physical Form Dark green crystals

Solubility Very soluble in water; slightly soluble to insoluble in ethanol; insoluble in xylene

UV-Visible (λ_{max}) 546 nm

Melting Point >250°C

Synthesis Synthetic methods^{1,2}

Major Applications Nanocomposite,³ recording materials,⁴ sol-gel matrix,⁵ decoder system,⁶ color filter,⁷ inks,⁸ paints,⁹ markers,¹⁰ highlighters,¹¹ corrosion inhibitors,¹² explosives,¹³ packaging system,¹⁴ textiles,¹⁵ hair dyes,¹⁶ make-up,¹⁷ cosmetics,¹⁸ food storage,¹⁹ dental bleaching,²⁰ detecting tumor cells,²¹ determine bacterial growth,²² cancer chemopreventive activity²³

Safety/Toxicity Genotoxicity,²⁴ oral toxicity,²⁵ neurotoxicity²⁶

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ACRIDINE

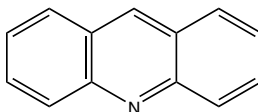
Other Names 10-Azaanthracene; 2,3-Benzoquinoline; 9-Azaanthracene; Benzo[b]quinoline; Dibenzo[b,e]pyridine; NSC 3408

CA Index Name Acridine

CAS Registry Number 260-94-6

Merck Index Number 122

Chemical Structure



Chemical/Dye Class Fluorescent, Acridine

Molecular Formula C₁₃H₉N

Molecular Weight: 179.22

pH Range: 5.2–6.6

Color Change at pH: Green fluorescence (5.2) to violet fluorescence (6.6)

pKa 5.50

Physical Form Yellow powder

Solubility Slightly soluble in boiling water; freely soluble in ethanol, ether

UV-Visible ($\lambda_{\max}$) 358 nm, 392 nm

Melting Point: 107–111°C

Boiling Point 346°C

Synthesis Synthetic methods^{1–13}

Major Applications Organic light-emitting diode,¹⁴ photoresists,¹⁵ nanosensors,¹⁶ fuel cells,¹⁷ memory device,¹⁸ semiconductors,¹⁹ information storage device,²⁰ liquid crystal displays,²¹ identification of product forgeries,²² inks,²³ adhesives,²³ textile,²⁴ hair dyes,²⁵ gene detection assay,²⁶ staining cells,²⁷ biosensors,²⁸ detecting nucleic acids,²⁹ proteins,²⁹ anti-HCV antibodies,³⁰ antibacterial,³¹ anti-amyloid agents,³² wound dressing materials,³³ vaccines against infection,³⁴ allergy³⁴ and cancer³⁴

Safety/Toxicity Acute toxicity,³⁵ bacterial toxicity,³⁶ carcinogenicity,³⁷ chronic toxicity,³⁸ cytotoxicity,³⁹ ecotoxicity,⁴⁰ genotoxicity,⁴¹ mutagenicity,⁴² phototoxicity,⁴³ phytotoxicity⁴⁴

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ALIZARIN RED

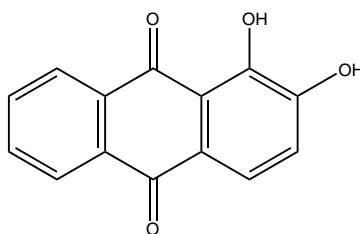
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CA Index Name 9,10-Anthracenedione, 1,2-dihydroxy-

CAS Registry Number 72-48-0

Merck Index Number 251

Chemical Structure



Chemical/Dye Class Miscellaneous, Anthraquinone

Molecular Formula C₁₄H₈O₄

Molecular Weight 240.21

pH Range 5.5–6.8;

10.1–12.1

Color Change at pH Yellow (5.5) to red (6.8)

Red (10.1) to purple (12.1)

pKa 6.77

Physical Form Orange powder

Solubility Virtually insoluble in water; moderately soluble in ethanol, soluble in benzene, toluene, xylene, pyridine, acetic acid

UV-Visible (λ_{max}) 567 nm, 609 nm

Melting Point 290°C

Boiling Point 430°C

Synthesis Synthetic methods^{1–8}

Major Applications Plasma displays,⁹ antireflective coatings,¹⁰ chemical-mechanical polishing,¹¹ photoreceptors,¹² glass coatings,¹³ paints,¹⁴ anticorrosion coatings,¹⁵ thermoplastics,¹⁶ wood coloring,¹⁷ textiles,¹⁸ pH sensor device,¹⁹ detergent,²⁰ hair dyes,²¹ darkening skin,²² cosmetics,²³ parasiticide,²⁴ antifungal agent²⁵

Safety/Toxicity Acute and subacute toxicity,²⁶ carcinogenicity,²⁷ environmental contaminants,²⁸ estrogenicity,²⁹ genotoxicity,³⁰ hypersensitivity,³¹ mutagenicity,³² photoinduced toxicity,³³ synergistic toxicity³⁴

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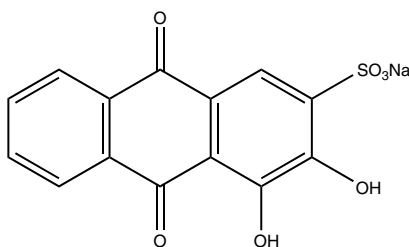
ALIZARIN RED S

Other Names 2-Anthraquinonesulfonic acid, 3,4-dihydroxy-, sodium salt; Acid Mordant Red SW; Acid Red Alizarine; Ahcoquinone Red S; Alizarin Carmine; Alizarin Red S; Alizarin S; Alizarine Carmine; Alizarine Carmine Indicator; Alizarine Red A; Alizarine Red AS; Alizarine Red Indicator; Alizarine Red S; Alizarine Red S sodium salt; Alizarine Red SW; Alizarine Red SZ; Alizarine Red W; Alizarine Red WA; Alizarine Red WS; Alizarine Red for Wool; Alizarine S; Alizarine S Extra Conc. A Export; Alizarine S Extra Pure A; Alizarinsulfonate; C.I. 58005; C.I. Mordant Red 3; Calcochrome Alizarine Red SC; Carnelio Rubine Lake; Chrome Red Alizarine; Diamond Red W; Ext D and C Red No. 7; Fenakrom Red W; Mitsui Alizarine Red S; Mordant Red 3; Oxanal Fast Red SW; Sodium 3,4-dihydroxyanthraquinone-2-sulfonate; Sodium alizarin-3-sulfonate; Sodium alizarinesulfonate; Sodium alizarinsulfonate

CA Index Name 2-Anthracenesulfonic acid, 9,10-dihydro-3,4-dihydroxy-9,10-dioxo-, monosodium salt

CAS Registry Number 130-22-3

Merck Index Number 8573

Chemical Structure

Chemical/Dye Class Anthraquinone

Molecular Formula $C_{14}H_7O_7SNa$

Molecular Weight 342.26

pH Range 3.5–6.5;

9.4–12.0

Color Change at pH Yellow (3.5) to red (6.5)

Orange (9.4) to violet (12.0)

pKa 4.5, 11

Physical Form Orange-yellow powder

Solubility Freely soluble in water; soluble in ethanol; insoluble in ether

UV-Visible (λ_{max}) 556 nm, 596 nm, 423 nm, 546 nm

Melting Point >250°C

Synthesis Synthetic methods¹⁻⁵

Major Applications Nanocomposite material,⁶ chemical mechanical polishing,⁷ optical fibers,⁸ display device,⁹ carbon nanotubes,¹⁰ textiles,¹¹ determination of aluminum,¹² iron,¹² copper,¹² manganese,¹³ zinc,¹³ calcium,¹⁴ magnesium,¹⁴ zirconium,¹⁵ hafnium,¹⁵ molybdenum,¹⁶ uranium,¹⁷ vanadium,¹⁸ detergents,¹⁹ hair dyes,²⁰ determination of proteins,²¹ clotrimazole,²² ketoconazole,²² piroxicam, and tenoxicam²³

Safety/Toxicity Carcinogenicity,²⁴ cytotoxicity,²⁵ genotoxicity,²⁵ toxicity to freshwater organisms,²⁶ environmental and pollutants²⁷

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ALIZARIN YELLOW GG

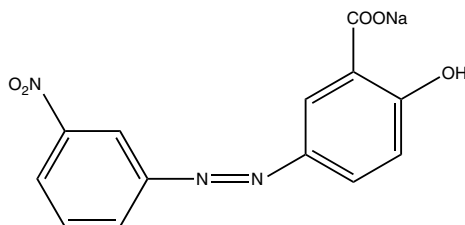
Other Names C.I. Mordant Yellow 1; C.I. Mordant Yellow 1, monosodium salt; Salicylic acid, 5-(*m*-nitrophenylazo)-, sodium salt; Acid Chrome Yellow 2GW; Acid Chrome Yellow GG; Alizarin Yellow; Alizarin Yellow G; Alizarin Yellow G sodium salt; Alizarin Yellow GG; Alizarine Yellow 2G; Alizarine Yellow AGP; Alizarine Yellow G; Alizarine Yellow GG; Alizarine Yellow GGW; Alizarine Yellow GM; Alizarine Yellow GR; Alizarol Yellow GW; Anthranol Chrome Yellow 2G; Anthranol Chrome Yellow 5GS; Atlantichrome Yellow 2G; Azochromol Yellow 5G; C.I. 14025; Calcochrome Yellow 2G; Chrome Fast Yellow RW; Chrome Yellow 2G; Chrome Yellow 2GR; Chromol Yellow G; Chromol Yellow N; Cromal Yellow M; Eniacromo Yellow G; Eriochromal Yellow 2G; Eriochrome Yellow 2G; Eriochrome Yellow GS; Fenakrom Yellow R; Hidachrome Yellow 2G; Hispacrom Yellow 2G; Hispacrom Yellow 2GR; Java Chrome Yellow GT; Java Unichrome Yellow GT; Kayaku Mordant Yellow GG; Magracrom Yellow GG; Metachrome Yellow; Metachrome Yellow RA; Metomega Chrome Yellow GM; Mitsui Chrome Yellow GG; Monochrome Yellow MG; Orthochrome Yellow GGW; Pontachrome Yellow GS; RV 1; Salicyl yellow; Salicylic acid, (*m*-nitrophenylazo)-, sodium salt; Showa Chrome Yellow GG; Sodium 5-(*m*-nitrophenylazo) salicylate; Sodium 5-[(3-nitrophenyl)-azo]-salicylate; Sodium *m*-nitrobenzeneazosalicylate; Solochrome Yellow WN; Sunchromine Yellow GG; Yodochrome Yellow GGN

CA Index Name Benzoic acid, 2-hydroxy-5-[(3-nitrophenyl)azo]-, monosodium salt

CAS Registry Number 584-42-9

Merck Index Number 5919

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula $C_{13}H_8N_3O_5Na$

Molecular Weight 309.22

pH Range 10.0–12.0

Color Change at pH Yellow (10.0) to orange (12.0)

Physical Form Yellow-orange powder

Solubility Soluble in water, methyl cellosolve; slightly soluble in ethanol, acetone

UV-Visible (λ_{max}) 362 nm

Melting Point >250°C

Synthesis Synthetic methods¹⁻³

Major Applications Optical engineering applications,⁴ sensors,⁵ making masks,⁶ electrorheological materials,⁷ surface treatment of copper,⁸ coloring zinc,⁹ aluminum,¹⁰ corrosion testing,¹¹ adhesive,¹² lubricants,¹³ textiles,¹⁴ food storage,¹⁵ determine bacterial growth,¹⁶ pharmaceutical preparations¹⁷

Safety/Toxicity Mutagenicity¹⁸

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ALIZARIN YELLOW R

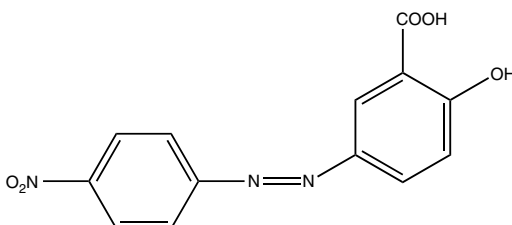
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CA Index Name Benzoic acid, 2-hydroxy-5-[(4-nitrophenyl)azo]-

CAS Registry Number 2243-76-7

Merck Index Number 255

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula $C_{13}H_9N_3O_5$

Molecular Weight 287.23

pH Range 10.0–12.1

Color Change at pH Yellow (10.0) to orange-red (12.1)

pKa 2.85

Physical Form Orange-brown powder

Solubility Soluble in water, ethanol; slightly soluble in acetone

UV-Visible ($\lambda_{\max}$) 385 nm

Melting Point 253–254°C (decompose)

Boiling Point (Calcd.) $571.4 \pm 50.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods¹⁻⁴

Major Applications Display device,⁵ photoresist,⁶ nanoparticles,⁷ sensors,^{8,9} image-recoring materials,¹⁰ photoconductive materials,^{11,12} photography,¹³ electrorheological materials,¹⁴ copying materials,¹⁵ optical engineering applications,¹⁶ monitoring oil degradation,¹⁷ lubricant,¹⁸ flame luminosity enhancing agent,¹⁹ coloring zinc,²⁰ method for polymerization of vinyl chloride,²¹ determination of OH groups on resins,²² cosmetics,²³ diapers,²⁴ food storage,²⁵ measurement of acidity in juice,²⁶ assay for aldehyde contents,²⁷ determination of albumin,²⁸ agent for plaque,²⁹ method for counting leukocytes,³⁰ antifungal agent³¹

Safety/Toxicity Toxicity,³² mutagenicity³³

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ALKALI BLUE

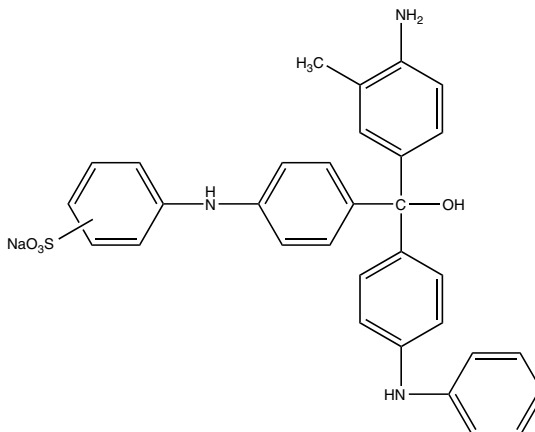
Other Names Alkali Blue 6B; Acid Blue 110

CA Index Name Benzenesulfonic acid, [[4-[(4-amino-3-methylphenyl)hydroxy[4-(phenylamino)phenyl]methyl]phenyl]amino]-, monosodium salt

CAS Registry Number 30586-13-1

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Triphenylmethane

Molecular Formula C₃₂H₂₈N₃O₄SNa

Molecular Weight 573.65

pH Range 9.4–14.0

Color Change at pH Blue-violet (9.4) to red-pink (14.0)

Physical Form Dark blue powder

Solubility Sparingly soluble in water; soluble in ethanol

UV-Visible (λ_{max}) 603 nm

Melting Point >250°C

Synthesis Synthetic methods¹

Major Applications Electrostatographic dry developers,¹ chelators for iron overload²

Safety/Toxicity No data available

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9-AMINO-6-CHLORO-2-METHOXYACRIDINE

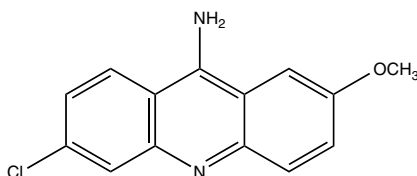
Other Names Acridine, 9-amino-6-chloro-2-methoxy-; 2-Methoxy-6-chloro-9-aminoacridine; 3-Chloro-7-methoxy-9-aminoacridine; 6-Chloro-9-amino-2-methoxyacridine; 9-Amino-3-chloro-7-methoxyacridine; 9-Amino-6-chloro-2-methoxyacridine; G 185; NSC 15300

CA Index Name 9-Acridinamine, 6-chloro-2-methoxy-

CAS Registry Number 3548-09-2

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula C₁₄H₁₁ClN₂O

Molecular Weight 258.70

pH Range 7.5–9.8

Color Change at pH Weak blue fluorescence (7.5) to strong blue fluorescence (9.8)

pKa 8.6

Physical Form Solid

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide, dimethyl sulfoxide

UV-Visible (λ_{max}) 412 nm

Melting Point >250°C

Boiling Point (Calcd.) 475.1 ± 35.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–7}

Major Applications Sensors,⁸ detection method for DNA amplification,⁹ inhibition of neurodegenerative diseases,¹⁰ RNA hydrolysis,^{11,12} fluorescent probes,^{13,14} primers for nucleic acid sequencing,¹⁵ synthesis of nucleic acids,¹⁶ antimalarial agent¹⁷

Safety/Toxicity Genotoxicity,¹⁸ mutagenicity^{19–21}

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5-AMINOSALICYLIC ACID

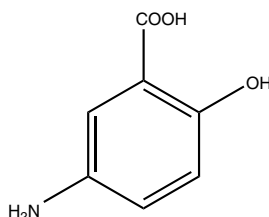
Other Names Salicylic acid, 5-amino-; 2-Hydroxy-5-aminobenzoic acid; 3-Carboxy-4-hydroxy-aniline; 5-ASA; 5-Amino-2-hydroxybenzoic acid; 5-Aminosalicylic acid; Asacol; Asacolit; Asacolon; Canasa; Claversal; Fisalamine; Ipocol; Lixacol; Mesacol; Mesalamine; Mesalazine; Mesasal; NSC 38877; Pentasa; Rowasa; Salofalk; Salozinal; *m*-Aminosalicylic acid

CA Index Name Benzoic acid, 5-amino-2-hydroxy-

CAS Registry Number 89-57-6

Merck Index Number 5904

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula $C_7H_7NO_3$

Molecular Weight 153.14

pH Range 3.1–4.4

Color Change at pH Non-fluorescence (3.1) to light green fluorescence (4.4)

pKa 2.74, 5.84

Physical Form White to pinkish crystals

Solubility Slightly soluble in cold water, ethanol; more soluble in hot water; soluble in hydrochloric acid

Melting Point 280°C (decompose)

Boiling Point (Calcd.) 403.9 ± 40.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–14}

Major Applications Detergent,¹⁵ hair dyes,¹⁶ prevention of colorectal cancer,¹⁷ treating inflammatory bowel disease,¹⁸ autoimmune disorders,¹⁹ gastrointestinal inflammation,²⁰ chemokine-mediated diseases,²¹ mucosal tissue disorder,²² sleep disorders,²³ rectoanal tenesmus,²⁴ ulcerative colitis²⁵

Safety/Toxicity Hepatotoxicity,^{26,27} cytotoxicity,^{27,28} nephrotoxicity,²⁹ risk of renal disease,³⁰ safety in pregnancy,³¹ side effects³²

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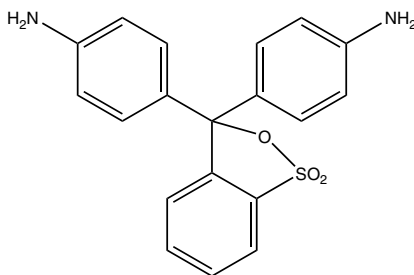
ANILINESULFONEPHTHALEIN

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CA Index Name Benzenamine, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)*bis*-

CAS Registry Number 4538-11-8

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Sulfonephthalein

Molecular Formula C₁₉H₁₆N₂O₃S

Molecular Weight 352.41

pH Range 1.32–1.92

11.75–12.53

Color Change at pH Yellow (1.32) to violet (1.92)

Violet (11.75) to yellow (12.53)

pKa 1.59, 12.26

Physical Form Leaflets with green lustre

Solubility Soluble in water, ethanol

Melting Point >250°C

Boiling Point (Calcd.) 570.4 ± 50.0°C Pressure: 760 Torr

Synthesis Synthetic method¹

Major Applications Phototranschromic materials²

Safety/Toxicity No data available

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ANTHRANILIC ACID

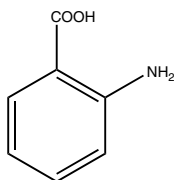
Other Names Anthranilic acid; α -Aminobenzoic acid; 1-Aminobenzene-2-carboxylic acid; 2-Aminobenzoic acid; 2-Carboxyaniline; 2-Carboxyphenylamine; NSC 144; NSC 40929; Vitamin L1; *o*-Aminobenzoic acid; *o*-Anthranilic acid; *o*-Carboxyaniline

CA Index Name Benzoic acid, 2-amino-

CAS Registry Number 118-92-3

Merck Index Number 422

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula $C_7H_7NO_2$

Molecular Weight 137.14

pH Range 1.5–3.0

4.5–6.0

12.5–14.0

Color Change at pH Non-fluorescence (1.5) light blue fluorescence (3.0)

Light blue fluorescence (4.5) to dark blue fluorescence (6.0)

Dark blue fluorescence (12.5) to non-fluorescence (14.0)

pKa 1.85, 4.95

Physical Form White to pale yellow crystalline powder

Solubility Sparingly soluble in cold water; freely soluble in hot water, ethanol, ether

Melting Point 144–147°C

Boiling Point (Calcd.) $311.9 \pm 25.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods^{1–5}

Major Applications Bottom antireflective coatings,⁶ semiconductor devices,⁷ inks,⁸ hair dyes,⁹ cosmetics,^{10,11} treatment of chronic inflammatory diseases,¹² depression¹³

Safety/Toxicity Acute oral toxicity,¹⁴ carcinogenicity,¹⁵ ecotoxicity,¹⁶ genotoxicity,¹⁷ mutagenicity,¹⁸ neurotoxicity,¹⁹ tumorigenicity²⁰

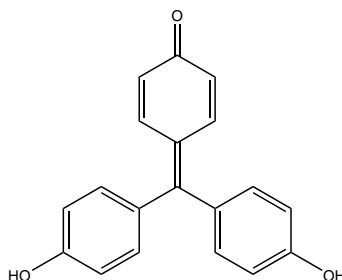
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AURIN

Other Names 2,5-Cyclohexadien-1-one, 4-[bis(*p*-hydroxyphenyl)methylene]-; Aurin; 4,4'-Dihydroxyfuchson; 4-(*p,p'*-Dihydroxybenzhydriidene)-2,5-cyclohexadien-1-one; 4-[Bis(*p*-hydroxyphenyl)methylene]-2,5-cyclohexadien-1-one; Aurin 555; Aurine; C.I. 43800; Corallin; Corallin Spirit Soluble; NSC 7805; Pararosolic acid; Rosalic acid; Spirit Aurine; *p*-Rosolic acid
CA Index Name 2,5-Cyclohexadien-1-one, 4-[bis(4-hydroxyphenyl)methylene]-
CAS Registry Number 603-45-2
Merck Index Number 881
Chemical Structure



Chemical/Dye Class Triphenylmethane

Molecular Formula C₁₉H₁₄O₃

Molecular Weight 290.31

pH Range 6.6–8.0

Color Change at pH Yellow (6.6) to red (8.0)

pKa 6.98

Physical Form Red crystals

Solubility Practically insoluble in water, benzene; freely soluble in ethanol

UV-Visible (λ_{max}) 534.6 nm, 479.5 nm, 482 nm

Melting Point 309°C (decompose)

Boiling Point (Calcd.) 543.0 ± 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–9}

Major Applications Antireflective coatings,¹⁰ thermochromic materials,¹¹ photoresists,² electrorheological materials,¹² film patterning,¹³ recording materials,¹⁴ lithium battery,¹⁵ semiconductors,¹⁶ printing materials,¹⁷ inks,¹⁸ corrosion inhibitors,¹⁹ adhesives,²⁰ drugs,²¹ detecting viable cells,²² treatment of Alzheimer's disease¹

Safety/Toxicity Toxic activity,²³ environmental toxicity,²⁴ cytopathogenicity²⁵

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B

BENZAURIN

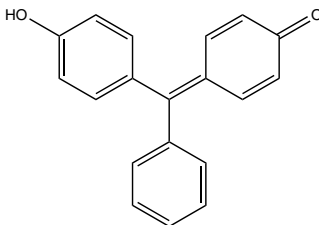
Other Names 2,5-Cyclohexadien-1-one, 4-(*p*-hydroxy- α -phenylbenzylidene)-; Benzaurin; NSC 55861; Phenolbenzein; Rosolic acid

CA Index Name 2,5-Cyclohexadien-1-one, 4-[(4-hydroxyphenyl)phenylmethylene]-

CAS Registry Number 569-60-8

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Benzein

Molecular Formula C₁₉H₁₄O₂

Molecular Weight 274.31

pH Range 6.0–7.6

Color Change at pH Yellow (6.0) to red (7.6)

pKa 9.28

Physical Form Orange-red crystals

Solubility Insoluble in water; soluble in ethanol

Melting Point >250°C

Boiling Point (Calcd.) 497.0 ± 45.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–5}

Major Applications Indicator⁶

Safety/Toxicity No data available

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BENZOPURPURIN 4B

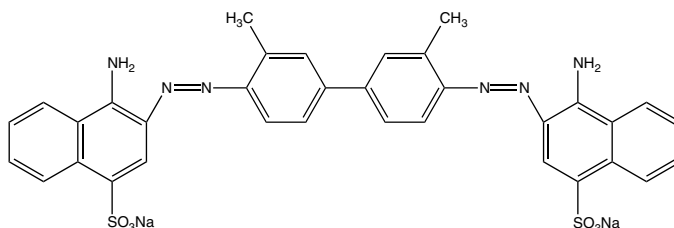
Other Names C.I. Direct Red 2; C.I. Direct Red 2, disodium salt; Amanil Purpurine 4B; Atul Direct Red 4B; Azamin 4B; Azocard Red 4B; Bencidal Purple 4B; Benzanil Purpurine 4B; Benzopurpurin 4B; Benzopurpurin B; Benzopurpurine 4B; Benzopurpurine 4BKX; Benzopurpurine 4BX; Brasilamina Red 4B; C.I. 23500; Calcomine Red 4BX; Chrome Leather Red 4B; Cotton Red 4B; Diacotton Benzopurpurine 4B; Diamine Purpurine 4B; Diaphtamine Purpurine 4B; Diazamine Purpurine 4B; Diazine Red 4B; Diazol Purpurine 4B; Diphenyl Red 4B; Diphenyl Red 4BS; Direct Purpurine 4B; Direct Purpurine M 4B; Direct Red 2; Direct Red 4A; Direct Red 4B; Direct Red DCB; Eclipse Red; Erie Benzo 4BP; Erie Red 4B; Fast Scarlet; Hispamin Red 4B; Kayaku Benzopurpurine 4B; Mitsui Benzopurpurine 4BX; Paper Red 4BS; Phenamine Purpurine 4B; Purpurin 4By; Purpurine 4B; Red 4B; Sultan 4B; Sultan Red 4B; Tertrodirect Red 4B

CA Index Name 1-Naphthalenesulfonic acid, 3,3'-[(3,3'-dimethyl[1,1'-biphenyl]-4,4'-diyl)*bis*(azo)]*bis*[4-amino-, disodium salt

CAS Registry Number 992-59-6

Merck Index Number 1101

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula C₃₄H₂₆N₆O₆S₂Na₂

Molecular Weight 724.73

pH Range 1.2–4.0

Color Change at pH Blue-violet (1.2) to red (4.0)

Physical Form Brown powder

Solubility Soluble in water, ethanol, acetone, sodium hydroxide, sulfuric acid

UV-Visible (λ_{max}) 500 nm

Melting Point >250°C

Synthesis Synthetic methods^{1–3}

Major Applications Liquid crystal displays,⁴ thin films,⁵ electronic devices,⁶ inks,⁷ lithographic printing plates,⁸ printing and dyeing applications,⁹ textiles,¹⁰ lubricants,¹¹ food storage,¹² microorganism staining agent,¹³ treatment of apolipoprotein E-related diseases,¹⁴ antifungal agent¹⁵

Safety/Toxicity Genotoxicity,¹⁶ mutagenicity^{17,18}

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BRILLIANT GREEN

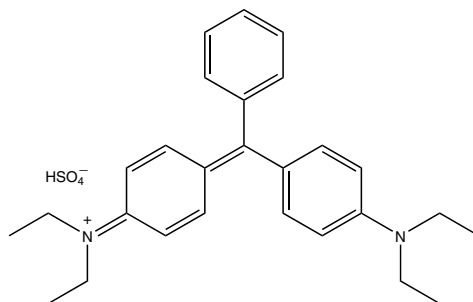
Other Names C.I. Basic Green 1; 12415 Green; ADC Brilliant Green Crystals; Aizen Diamond Green GH; Aizen Malachite Green GH; Astra Diamond Green GX; Astrazon Green D; Avon Green A 4379; Basic Bright Green; Basic Bright Green Sulfate; Basic Brilliant Green; Basic Green 1; Basic Green V; Brilliant Green; Brilliant Green B; Brilliant Green BP; Brilliant Green BP Crystals; Brilliant Green BPC; Brilliant Green Crystals; Brilliant Green Crystals H; Brilliant Green DSC; Brilliant Green G; Brilliant Green GX; Brilliant Green Lake; Brilliant Green P; Brilliant Green Special; Brilliant Green Sulfate; Brilliant Green WP Crystals; Brilliant Green Y; Brilliant Green YN; Brilliant Green YNS; Brilliant Lake Green Y; Brilliant green aseptic; C.I. 42040; Calcozine Brilliant Green G; Deorlene Green JJO; Diamond Green G; Diamond Green GH; Ethyl green; Fast Green J; Fast Green JJO; Green EN; Hidaco Brilliant Green; Malachite Green G; Mitsui Brilliant Green GX; NSC 5011; Resplendency Green; Solid Green; Tertrophenes Brilliant Green G; Tokyo Aniline Brilliant Green

CA Index Name Ethanaminium, *N*-[4-[[4-(diethylamino)phenyl]phenylmethylene]-2,5-cyclohexadien-1-ylidene]-*N*-ethyl-, sulfate

CAS Registry Number 633-03-4

Merck Index Number 1374

Chemical Structure



Chemical/Dye Class Triphenylmethane

Molecular Formula $C_{27}H_{34}N_2O_4S$

Molecular Weight 482.63

pH Range 0.0–2.6

Color Change at pH Yellow (0.0) to green (2.6)

Physical Form Green crystals

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 625 nm, 428 nm

Melting Point 210°C (decompose)

Synthesis Synthetic methods^{1–10}

Major Applications Black matrix,¹¹ color filter,¹¹ photoresists,¹² sensors,¹³ inks,¹⁴ rodenticide,¹⁵ hair dyes,¹⁶ cosmetics,¹⁷ detecting dental carious tissue,¹⁸ *Escherichia coli*,¹⁹ antimalarial agent,²⁰ wound dressing material,²¹ treatment of cancer,²² medical devices²³

Safety/Toxicity Toxicity to aquatic animals,²⁴ carcinogenicity²⁵

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BRILLIANT YELLOW

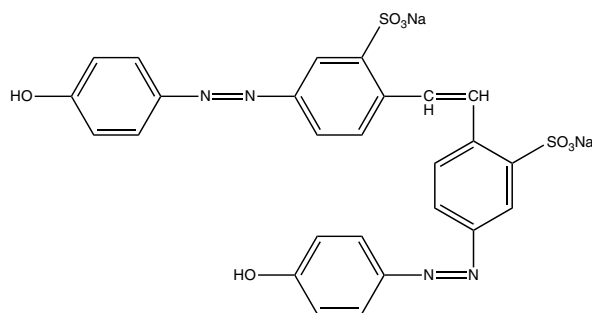
Other Names Brilliant Yellow C; C.I. Direct Yellow 4; C.I. Direct Yellow 4, disodium salt; Benzo Brilliant Yellow; Brilliant Fast Yellow G2N; Brilliant Paper Yellow; Brilliant Paper Yellow C; Brilliant Paper Yellow P; Brilliant Yellow; Brilliant Yellow (indicator); C.I. 24890; Calcomine Brilliant Paper Yellow; Chlorazol Brilliant Yellow 3G; Diaphtamine Brilliant Fast Yellow 3G; Diazol Brilliant Yellow N; Direct Brilliant Yellow G; Direct Yellow 4; Fenamin Yellow 3G; Kayaku Direct Yellow G; Nippon Brilliant Yellow G; Paper Yellow 3GX; Paper Yellow 3GXA; Paper Yellow CB; Tertrodirect Yellow B; Trisulfon Paper Yellow

CA Index Name Benzenesulfonic acid, 2,2'-(1,2-ethenediyl)bis[5-[(4-hydroxyphenyl)azo]-, disodium salt

CAS Registry Number 3051-11-4

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula $C_{26}H_{18}N_4O_8S_2Na_2$

Molecular Weight 624.56

pH Range 6.4–8.0

Color Change at pH Yellow (6.4) to red-orange (8.0)

Physical Form Orange powder

Solubility Soluble in water; slightly soluble in ethanol, acetone

UV-Visible (λ_{max}) 497 nm

Melting Point >250°C

Synthesis Synthetic methods^{1–3}

Major Applications Display device,⁴ sensors,^{5,6} photochromic materials,⁷ inks,⁸ detergent,⁹ cosmetics,¹⁰ biosensors,¹¹ assay for enzyme activity,¹² antifungal agent,¹³ antiAIDS agent¹⁴

Safety/Toxicity No data available

References

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BROMOCHLOROPHENOL BLUE

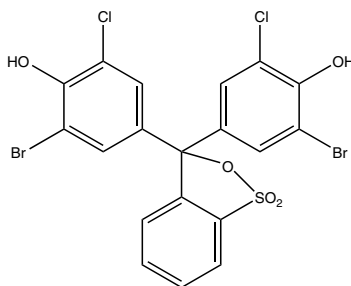
Other Names Bromochlorophenol blue; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-6-chloro-, S,S-dioxide; *o*-Toluenesulfonic acid, α,α -bis(3-bromo-5-chloro-4-hydroxyphenyl)- α -hydroxy-, γ -sultone; 3H-2,1-Benzoxathiole, phenol deriv.; Bromchlorophenol blue; NSC 7816

CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-6-chloro-

CAS Registry Number 2553-71-1

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula $C_{19}H_{10}Br_2Cl_2O_5S$

Molecular Weight 581.06

pH Range 3.0–4.6

Color Change at pH Yellow (3.0) to purple (4.6)

pKa 6.05

Physical Form Violet-pink powder

Solubility Sparingly soluble in water; soluble in ethanol

UV-Visible (λ_{max}) 590 nm

Melting Point 230°C (decompose)

Boiling Point (Calcd.) $602.9 \pm 55.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic method¹

Major Applications Display device,² pH sensors,³ inks,⁴ photoreceptors,⁵ lithographic plates,⁶ photographic materials,⁷ determination of surfactants,^{8,9} lubricants,¹⁰ food shelf life,^{11,12} in protein assays,¹³ vaginal infection test,¹⁴ detecting proteins^{15,16}

Safety/Toxicity No data available

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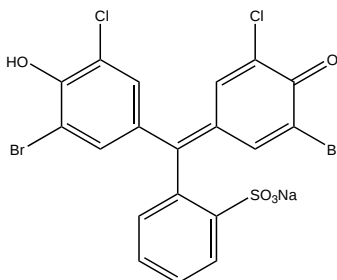
BROMOCHLOROPHENOL BLUE, SODIUM SALT

Other Names Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-6-chloro-, S,S-dioxide, monosodium salt; 3H-2,1-Benzoxathiole, phenol deriv.

CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-6-chloro-, monosodium salt

CAS Registry Number 102185-52-4

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Sulfonephthalein

Molecular Formula C₁₉H₉Br₂Cl₂O₅SNa

Molecular Weight 580.07

pH Range 3.0–4.6

Color Change at pH Yellow (3.0) to purple (4.6)

pKa 6.05

Physical Form Black powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 590 nm

Melting Point >250°C

Synthesis Synthetic method¹

Major Applications Chemical probe²

Safety/Toxicity No data available

References

1. Sergeev, G. M.; Korenman, I. M. Composition and stability of complexes of thorium with bromphenol and bromchlorophenol blue. *Zh. Neorg. Khim.* **1978**, 23, 121–125; *Chem. Abstr.* **1978**, 88, 95605.
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BROMOCRESOL GREEN

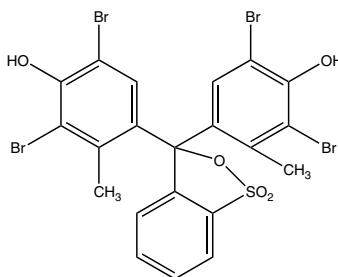
Other Names Bromocresol green; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dibromo-3-methyl-, S,S-dioxide; *m*-Cresol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dibromo-, S,S-dioxide; *o*-Toluenesulfonic acid, α,α -bis(3,5-dibromo-4-hydroxy-*o*-tolyl)- α -hydroxy-, γ -sultone; 3H-2,1-Benzoxathiole, phenol deriv.; 3',3'',5',5''-Tetrabromo-*m*-cresolsulfonephthalein; BCG; Bromocresol green; NSC 7817; Tetrabromo-*m*-cresolphthalein sulfone

CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dibromo-3-methyl-

CAS Registry Number 76-60-8

Merck Index Number 1386

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula C₂₁H₁₄Br₄O₅S

Molecular Weight 698.01

pH Range 3.8–5.4

Color Change at pH Yellow (3.8) to blue-green (5.4)

pKa 4.7, 4.6

Physical Form Slightly yellowish-brownish crystals

Solubility Sparingly soluble in water; soluble in ethanol, ether, ethyl acetate

UV-Visible (λ_{max}) 423 nm, 444 nm, 617 nm

Melting Point 218–219°C

Boiling Point (Calcd.) 626.0 $\pm$ 55.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–3}

Major Applications Sol-gel matrix,^{4,5} fuel cells,⁶ sensors,⁷ display device,⁸ inks,⁹ paints,¹⁰ one-step tester for ammonia,¹¹ packaging system,¹² textiles,¹³ cleansing products,¹⁴ detergents,¹⁵ cosmetics,¹⁶ diapers,¹⁷ identifying fresh and stale rice,¹⁸ monitoring fish spoilage,¹⁹ detecting carbohydrates,²⁰ lactating acid bacteria,²¹ treating neoplasms,²² cancer,²³ vaginal infection test method,²⁴ psychoactive drugs,²⁵ dental materials²⁶

Safety/Toxicity Effects in the environment,²⁷ cholestasis,²⁸ mutagenicity²⁹

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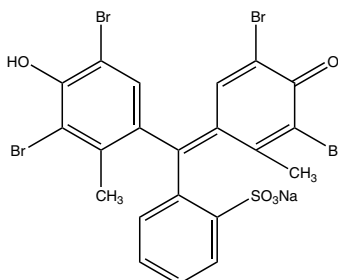
BROMOCRESOL GREEN, SODIUM SALT

Other Names Phenol, 4,4'-(3H-1,2-benzoxathiol-3-ylidene)bis[2,6-dibromo-3-methyl-, S,S-dioxide, monosodium salt; 3H-1,2-Benzoxathiole, phenol deriv.

CA Index Name Phenol, 4,4'-(2,2-dioxido-3H-1,2-benzoxathiol-3-ylidene)bis[2,6-dibromo-3-methyl-, monosodium salt

CAS Registry Number 62625-32-5

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Sulfonephthalein

Molecular Formula C₂₁H₁₃Br₄O₅Na

Molecular Weight 720.02

pH Range 3.8–5.4

Color Change at pH Yellow (3.8) to blue-green (5.4)

pKa 4.6

Physical Form Greenish-black crystalline powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 617 nm, 400 nm

Melting Point 230°C (decompose)

Synthesis Synthetic method¹

Major Applications Colloidal pigments²

Safety/Toxicity No data available

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1. Orndorff, W. R.; Purdy, A. C. Meta-cresolsulfonephthalein, 3,6-dimethylsulfonefluoran and some of their derivatives. *J. Am. Chem. Soc.* **1926**, *48*, 2212–2221.
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BROMOCRESOL PURPLE

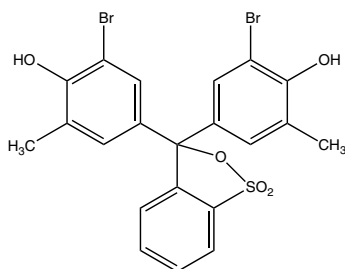
Other Names Bromocresol purple; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-6-methyl-, S,S-dioxide; *o*-Cresol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[6-bromo-, S,S-dioxide; *o*-Toluenesulfonic acid, α,α -bis(5-bromo-4-hydroxy-*m*-tolyl)- α -hydroxy-, γ -sultone; 3H-2,1-Benzoxathiole, phenol deriv.; Bromcresol purple; NSC 374134

CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-6-methyl-

CAS Registry Number 115-40-2

Merck Index Number 1387

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula $C_{21}H_{16}Br_2O_5S$

Molecular Weight 540.22

pH Range 5.2–6.8

Color Change at pH Yellow (5.2) to purple (6.8)

pKa 6.21, 6.3, 6.4

Physical Form Orange-yellow to brick red powder

Solubility Sparingly soluble in water; soluble in ethanol, ether, ethyl acetate

UV-Visible (λ_{max}) 419 nm, 433 nm, 591 nm

Melting Point 241.5°C

Boiling Point (Calcd.) $590.2 \pm 50.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods¹

Major Applications Waveguides,² fuel cells,³ sensors,⁴ sol-gel technology,⁵ display device,⁶ falsification-proof security paper,⁷ paints,⁸ detergents,⁹ identifying fresh and stale rice,¹⁰ detecting lactic acid bacteria,¹¹ dental materials,¹² vaginal infection test method¹³

Safety/Toxicity Mutagenicity,¹⁴ toxicity¹⁵

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BROMOCRESOL PURPLE, SODIUM SALT

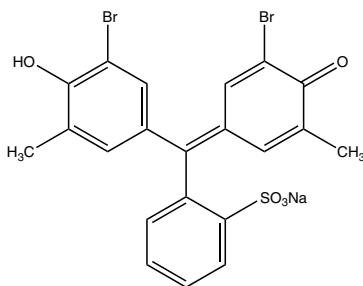
Other Names Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-6-methyl-, S,S-dioxide, monosodium salt; 3H-2,1-Benzoxathiole, phenol deriv.

CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-6-methyl-, monosodium salt

CAS Registry Number 62625-30-3

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula C₂₁H₁₅Br₂O₅SNa

Molecular Weight 562.22

pH Range 5.2–6.8

Color Change at pH Yellow (5.2) to purple (6.8)

pKa 6.3, 6.12

Physical Form Brownish-black crystalline powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 585 nm, 379 nm

Melting Point 255°C (decompose)

Synthesis Synthetic method¹

Major Applications Study properties of silicon dioxide films¹

Safety/Toxicity No data available

Reference

1. Murashkevich, A. N.; Vashina, V. G.; Zharskii, I. M. Structural-sorption properties of films of SiO₂. *Seryya Khim. Navuk* **2002**, 10–16; *Chem. Abstr.* **2002**, 137, 68531.

BROMOPHENOL BLUE

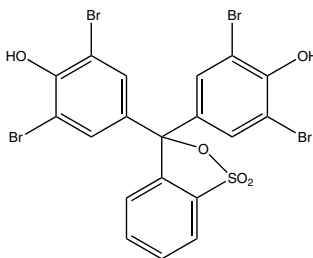
Other Names Bromophenol Blue; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dibromo-, S,S-dioxide; 3H-2,1-Benzoxathiole, phenol deriv.; 3',3'',5',5''-Tetrabromophenolsulfophthalein; Albutest; Bromphenol blue; NSC 7818; Tetrabromophenolsulfophthalein

CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dibromo-

CAS Registry Number 115-39-9

Merck Index Number 1444

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula C₁₉H₁₀Br₄O₅S

Molecular Weight 669.96

pH Range 3.0–4.6

Color Change at pH Yellow (3.0) to blue-purple (4.6)

pKa 4.0, 3.85, 3.6

Physical Form Yellowish-brownish powder

Solubility Sparingly soluble in water; soluble in ethanol, methanol, benzene

UV-Visible (λ_{max}) 598 nm, 592 nm, 436 nm, 422 nm, 273 nm

Melting Point 279°C (decompose)

Boiling Point (Calcd.) 605.6 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–5}

Major Applications Nanotechnology,⁶ semiconductors,⁷ sol-gel matrix,⁸ fuel cells,⁹ display device,¹⁰ paints,¹¹ packaging system,¹² diapers,¹³ contact lens,¹⁴ determining nucleic acids,¹⁵ mucin in saliva,¹⁶ water alkalinity,¹⁷ preserving genetic materials,¹⁸ detecting bacteria,¹⁹ vaginal infection test method²⁰

Safety/Toxicity Toxicology,²¹ mutagenicity,²² toxicity²³

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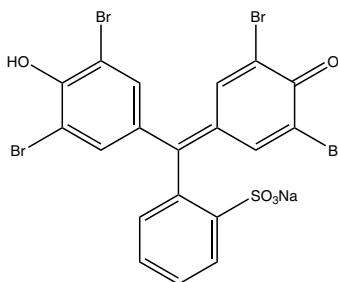
BROMOPHENOL BLUE, SODIUM SALT

Other Names Phenol, 4,4'-(3H-1,2-benzoxathiol-3-ylidene)bis[2,6-dibromo-,S,S-dioxide, mono-sodium salt; 3H-1,2-Benzoxathiole, phenol deriv.

CA Index Name Phenol, 4,4'-(2,2-dioxido-3H-1,2-benzoxathiol-3-ylidene)bis[2,6-dibromo-, mono-sodium salt

CAS Registry Number 62625-28-9

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Sulfonephthalein

Molecular Formula C₁₉H₉Br₄O₅SNa

Molecular Weight 691.97

pH Range 3.0–4.6

Color Change at pH Yellow (3.0) to blue (4.6)

pKa 4.0, 3.85, 3.6

Physical Form Blue-black crystalline powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 589 nm, 383 nm

Melting Point >250°C

Synthesis Synthetic methods^{1–3}

Major Applications Recording materials⁴

Safety/Toxicity No data available

References

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BROMOPHENOL RED

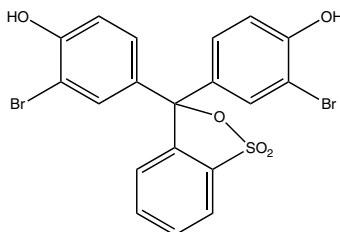
Other Names Bromophenol red; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)*bis*[2-bromo-, S,S-dioxide; *o*-Toluenesulfonic acid, α,α -*bis*(3-bromo-4-hydroxyphenyl)- α -hydroxy-, γ -sultone; 3H-2,1-Benzoxathiole, phenol deriv.; Bromophenol red

CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)*bis*[2-bromo-

CAS Registry Number 2800-80-8

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula C₁₉H₁₂Br₂O₅S

Molecular Weight 512.17

pH Range 5.2–6.8

Color Change at pH Yellow (5.2) to red (6.8)

pKa 6.51

Physical Form Reddish-brown powder

Solubility Sparingly soluble in water; soluble in ethanol

UV-Visible (λ_{max}) 574 nm

Melting Point >250°C

Boiling Point (Calcd.) 586.8 $\pm$ 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Sensors,^{3,4} sol-gel matrix,⁵ recording materials,⁶ thermochromic materials,⁷ inks,⁸ paints,⁹ alloy coatings,¹⁰ lubricants,¹¹ soaps,¹² cosmetics,¹³ identifying fresh & stale rice,¹⁴ determining acidity in wine,¹⁵ food storage,¹⁶ determination of bacterial growth,¹⁷ anti-amyloid agents,^{18,19} evaluating dental caries activity,^{20,21} determination of *Streptococci* in human saliva,²² diagnosis of enterohemorrhagic *Escherichia coli*,²³ treatment of acute leukemia²⁴

Safety/Toxicity No data available

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BROMOTHYMOL BLUE

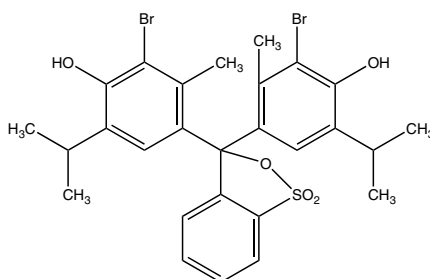
Other Names Bromothymol blue; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-3-methyl-6-(1-methylethyl)-, S,S-dioxide; Thymol, 6,6'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-, S,S-dioxide; 3H-2,1-Benzoxathiole, phenol deriv.; 3,3'-Dibromothymolsulfonphthalein; 3,3'-Dibromothymolsulfophthalein; Bromthymol blue; Dibromothymolsulfophthalein; NSC 7819

CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2-bromo-3-methyl-6-(1-methylethyl)-

CAS Registry Number 76-59-5

Merck Index Number 1445

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula $C_{27}H_{28}Br_2O_5S$

Molecular Weight 624.38

pH Range 6.0–7.6

Color Change at pH Yellow (6.0) to blue (7.6)

pKa 7.0, 7.1

Physical Form Light pink or cream colored powder

Solubility Sparingly soluble in water, benzene; soluble in ethanol, ether; insoluble in petroleum ether

UV-Visible (λ_{max}) 420 nm, 435 nm, 620 nm

Melting Point 201°C

Boiling Point (Calcd.) $614.3 \pm 55.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods^{1–5}

Major Applications Sol-gel matrix,⁶ fuel cells,⁷ optical sensors,⁸ combustion gas detection system,⁹ paints,¹⁰ toys,¹¹ cleaning products,¹² detergents,¹³ textiles,¹⁴ food freshness sensor,¹⁵ identifying fresh and stale rice,¹⁶ wheat,¹⁷ detecting microorganisms,¹⁸ bacterial growth,¹⁹ psychoactive drug,²⁰ dental materials²¹

Safety/Toxicity Toxicity²²

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BROMOTHYMOL BLUE, SODIUM SALT

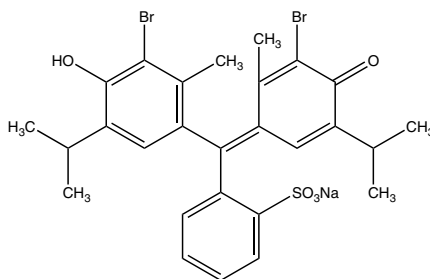
Other Names Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)*bis*[2-bromo-3-methyl-6-(1-methylethyl)-, S,S-dioxide, monosodium salt; 3H-2,1-Benzoxathiole, phenol deriv.; Bromthymol blue sodium

CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)*bis*[2-bromo-3-methyl-6-(1-methylethyl)-, monosodium salt

CAS Registry Number 34722-90-2

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula C₂₇H₂₇Br₂O₅SNa

Molecular Weight 646.38

pH Range 6.0–7.6

Color Change at pH Yellow (6.0) to blue (7.6)

pKa 7.0, 7.1

Physical Form Orange-brown powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 615 nm, 392 nm

Melting Point >250°C

Synthesis Synthetic method^{1,2}

Major Applications Lithium battery,³ textiles,² antagonists⁴

Safety/Toxicity No data available

References

1. Orndorff, W. R.; Cornwell, T. K. Thymolsulfonephthalein, the intermediate acid, 4'-hydroxy-3'-isopropyl-6'-methyl-benzoylbenzene-2-sulfonic acid and some of their derivatives. *J. Am. Chem. Soc.* **1926**, *48*, 981–993.
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BROMOXYLENOL BLUE

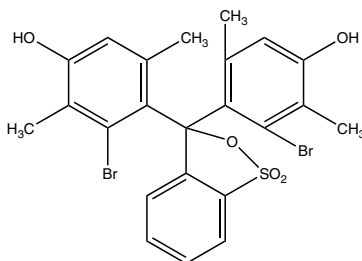
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CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[3-bromo-2,5-dimethyl-

CAS Registry Number 40070-59-5

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula C₂₃H₂₀Br₂O₅S

Molecular Weight 568.27

pH Range 6.0–7.6

Color Change at pH Yellow (6.0) to blue (7.6)

pKa 7.0

Physical Form Violet powder

Solubility Slightly soluble in water, ethanol; soluble in ethyl acetate, acetone

UV-Visible (λ_{max}) 417 nm

Melting Point 218°C (decompose)

Boiling Point (Calcd.) 642.8 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic method¹

Major Applications Optical lenses,² sol-gel matrix,³ inks,⁴ paints,⁴ toys,⁴ lubricants,⁵ cosmetics,⁶ food storage,⁷ microorganism detector,⁸ determination of drugs,⁹ diagnosis of multiple diseases¹⁰

Safety/Toxicity No data available

References

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C

CALCEIN

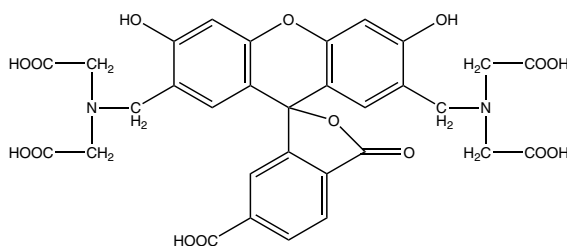
Other Names Fluorescein, 2',7'-bis[[bis(carboxymethyl)amino]methyl]-; Spiro[isobenzofuran-1(3H),9'-[9H]xanthene], glycine derivative; 2,7-Bis[*N,N*-bis(carboxymethyl)aminomethylene]-fluorescein; Acetic acid, [(3',6'-dihydroxy-2',7'-fluorandiyl)bis-(methylenenitrilo)]tetra-; Calcein; Fluorescein complexon; Fluorexon; NSC 298193; Oftasceine

CA Index Name Glycine, *N,N'*-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-2',7'-diyl)bis(methylene)]bis[*N*-(carboxymethyl)-

CAS Registry Number 1461-15-0

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula C₃₀H₂₆N₂O₁₃

Molecular Weight 622.53

pH Range 6.0–7.2

Color Change at pH Weak green fluorescence (6.0) to strong green fluorescence (7.2)

pKa 6.67

Physical Form Orange powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 494 nm

Melting Point >250°C

Boiling Point (Calcd.) 952.7 ± 65.0°C Pressure: 760 Torr

Synthesis Synthetic methods¹⁻⁶

Major Applications Chemical-mechanical polishing,^{7,8} stabilizing liposomes,⁹ cell motility assay,¹⁰ detecting nucleic acids,¹¹ virus,¹² screening safety of gastric mucosa,¹³ MDR inhibitors,¹⁴ drug delivery,¹⁵ imaging atherosclerotic plaque¹⁶

Safety/Toxicity Cytotoxicity,¹⁷ exitotoxicity¹⁸

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CALMAGITE

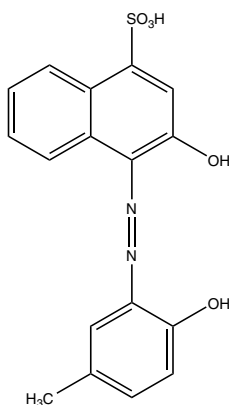
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CA Index Name 1-Naphthalenesulfonic acid, 3-hydroxy-4-[(2-hydroxy-5-methylphenyl)azo]-

CAS Registry Number 3147-14-6

Merck Index Number 1718

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula C₁₇H₁₄N₂O₅S

Molecular Weight 358.37

pH Range 7.1–9.1

Color Change at pH Red (7.1) to blue (9.1)

pKa 8.1

Physical Form Red-blackish crystals

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 610 nm

Melting Point 300°C

Synthesis Synthetic methods^{1,2}

Major Applications Nanoparticles,³ cleaning microelectronic substrates,⁴ sensors,⁵ photographic materials,⁶ recording materials,⁷ water hardness measurement,⁸ indicator for calcium and magnesium,⁹ determination of vanadium,¹⁰ medical component,¹¹ measuring magnesium in biological fluids,¹² diagnosis of diseases caused by elemental imbalance,¹³ treatment of thrombocytopenia,¹⁴ urine analysis test strip¹⁵

Safety/Toxicity No data available

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CARBAZOL YELLOW

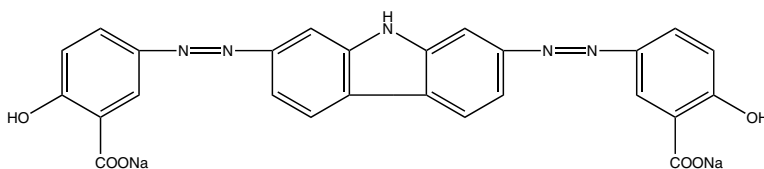
Other Names Salicylic acid, 5,5'-[carbazole-2,7-diylbis(azo)]di-, disodium salt; C.I. 25700; Carbazol Yellow

CA Index Name Benzoic acid, 3,3'-[9H-carbazole-2,7-diylbis(azo)]bis[6-hydroxy-, disodium salt

CAS Registry Number 6411-46-7

Merck Index Number Not listed

Chemical Structur



Chemical/Dye Class Azo

Molecular Formula $C_{26}H_{15}N_5O_6Na_2$

Molecular Weight 539.40

pH Range 12.0–14.0

Color Change at pH Yellow (12.0) to red (14.0)

pKa 13.7

Physical Form Yellow crystals

Solubility Soluble in water, ethanol

Melting Point >250°C

Synthesis No data available

Major Applications No data available

Safety/Toxicity No data available

References No reference available

5-CARBOXYFLUORESCEIN

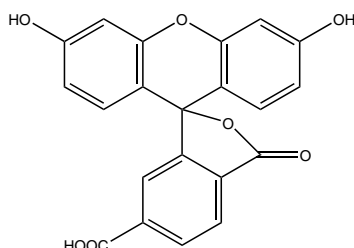
Other Names 5-Carboxyfluorescein; FAM; FAM (dye); FAM 494/520

CA Index Name Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid,3',6'-dihydroxy-3-oxo-

CAS Registry Number 76823-03-5

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula C₂₁H₁₂O₇

Molecular Weight 376.32

pH Range 6.0–7.2

Color Change at pH Weak green fluorescence (6.0) to strong green fluorescence (7.2)

pKa 3.3, 4.6, 6.4, 7.0

Physical Form Solid

Solubility Soluble in water, *N,N*-dimethylformamide

UV-Visible (λ_{max}) 492 nm

Melting Point >250°C

Boiling Point (Calcd.) 725.2 ± 60.0°C Pressure: 760 Torr

Synthesis Synthetic methods¹⁻³

Major Applications Fluorescent probe,⁴ diagnosis of cancer,⁵ leukemia,⁶ colorectal cancer,⁷ polynucleotide,⁸ bacteria,⁹ pathogens,¹⁰ nucleic acid,¹¹ hepatitis A virus,¹² dengue virus,¹³ herpes simplex virus,¹⁴ gene,¹⁵ HIV type,¹⁶ cardiovascular risk factor¹⁷

Safety/Toxicity Genotoxicity¹⁸

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6-CARBOXYFLUORESCEIN

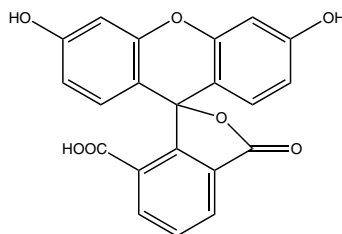
Other Names Spiro[phthalan-1,9'-xanthene]-6-carboxylic acid,3',6'-dihydroxy-3-oxo-; Terephthalic acid, (3,6,9-trihydroxyxanthen-9-yl)-, γ -lactone; 6-Carboxyfluorescein; 6-FAM; 6-carboxyfluorescein; Fluorescein, 6-carboxy-

CA Index Name Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid,3',6'-dihydroxy-3-oxo-

CAS Registry Number 3301-79-9

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula $C_{21}H_{12}O_7$

Molecular Weight 376.32

pH Range 6.0–7.2

Color Change at pH Weak green fluorescence (6.0) to strong green fluorescence (7.2)

pKa 3.3, 4.6, 6.4, 7.0

Physical Form Solid

Solubility Soluble in water, *N,N*-dimethylformamide

UV-Visible (λ_{max}) 492 nm

Melting Point $>360^\circ\text{C}$

Boiling Point (Calcd.) $736.4 \pm 60.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Diagnosis of hematologic cancer,³ nongastric diseases,⁴ detection of genetically modified wheat,⁵ chromosomes,⁶ gene expression,⁷ nucleic acid,⁸ hepatitis A virus,⁹ avian influenza virus subtype H5 and H5N1,¹⁰ SARS virus,¹¹ herpes simplex virus¹²

Safety/Toxicity Cytotoxicity,¹³ genotoxicity,¹⁴ immunotoxicity¹⁵

References

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5-CARBOXYFLUORESC EIN DIACETATE

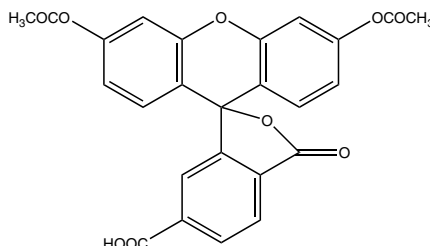
Other Names 5-Carboxyfluorescein diacetate

CA Index Name Spiro[isobenzofuran-1(3H),9′-[9H]xanthene]-5-carboxylic acid,3′,6′-bis(acetyloxy)-3-oxo-

CAS Registry Number 79955-27-4

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula C₂₅H₁₆O₉

Molecular Weight 460.39

pH Range 6.0–7.2

Color Change at pH Weak green fluorescence (6.0) to strong green fluorescence (7.2)

pKa 6.4

Physical Form Solid

Solubility Insoluble in water; soluble in dimethyl sulfoxide

UV-Visible (λ_{max}) <300 nm

Melting Point >250°C

Boiling Point (Calcd.) 693.1 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–9}

Major Applications Sensors,¹⁰ method for measuring bacteria,¹¹ detecting intracellular pH in yeast,¹² determination of extracellular and intracellular pH of microorganisms,¹³ detecting living cells,^{14,15} identification of cancerous cells,¹⁶ method for assessing microorganism viability,¹⁷ determining proliferative activities in tumor tissues,¹⁸ measuring the growth of keratinocytes,¹⁹ antifungal agent,^{20,21} neurodegenerative disorders,²² antineoplastic drugs²³

Safety/Toxicity No data available

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6-CARBOXYFLUORESC EIN DIACETATE

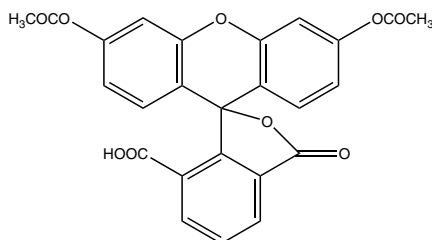
Other Names Spiro[phthalan-1,9'-xanthene]-6-carboxylic acid, 3',6'-dihydroxy-3-oxo-, diacetate; Terephthalic acid, (3,6,9-trihydroxyxanthen-9-yl)-, γ -lactone, diacetate; 6-Carboxyfluorescein diacetate

CA Index Name Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid,3',6'-bis (acetyloxy)-3-oxo-

CAS Registry Number 3348-03-6

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula $C_{25}H_{16}O_9$

Molecular Weight 460.39

pH Range 6.0–7.2

Color Change at pH Weak green fluorescence (6.0) to strong green fluorescence (7.2)

pKa 6.4

Physical Form Solid

Solubility Insoluble in water; soluble in dimethyl sulfoxide

UV-Visible (λ_{max}) <300 nm

Melting Point 152–153°C

Boiling Point (Calcd.) 701.6 $\pm$ 60.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–3}

Major Applications Fluorescent probes,⁴ detecting cells,⁵ microorganisms,⁵ yeasts,⁶ antifungal agent,⁷ antibacterials agent⁸

Safety/Toxicity Plasmid mobility of xenobiotics,⁹ retinal toxicity¹⁰

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5(6)-CARBOXYFLUORESC EIN DIACETATE SUCCINIMIDYL ESTER

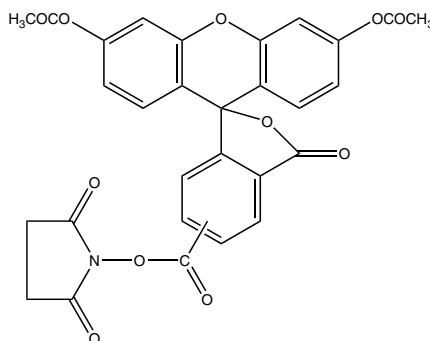
Other Names Spiro[isobenzofuran-1(3H),9'-[9H]xanthene], 2,5-pyrrolidinedione derivative; 5-(6)-Carboxyfluorescein diacetate succinimidyl ester

CA Index Name 2,5-Pyrrolidinedione, 1-[[[3',6'-bis(acetyloxy)-3-oxospiro-[isobenzofuran-1(3H),9'-[9H]xanthen]-5(or 6)-yl]carbonyl]oxy]-

CAS Registry Number 150347-59-4

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula C₂₉H₁₉NO₁₁

Molecular Weight 557.47

pH Range 6.0–7.2

Color Change at pH Weak green fluorescence (6.0) to strong green fluorescence (7.2)

pKa 6.45

Physical Form Solid

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide, dimethyl sulfoxide

UV-Visible (λ_{max}) <300

Melting Point >250°C

Synthesis Synthetic methods^{1–3}

Major Applications Diagnosis of cancer,⁴ restricting HIV replication,⁵ antiinflammatory agent,⁶ detecting bacteria,⁷ cell proliferation assays⁸

Safety/Toxicity No data available

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5-CARBOXYNAPHTHOFLUORESCIN

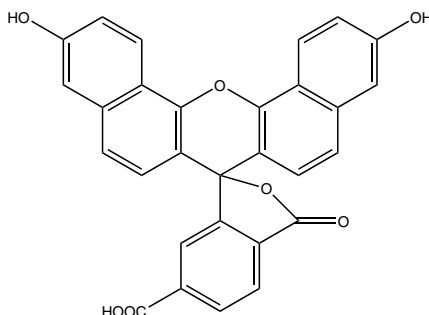
Other Names 5-Carboxynaphthofluorescein

CA Index Name Spiro[7H-dibenzo[c,h]xanthene-7,1'(3'H)-isobenzofuran]-5'-carboxylic acid, 3,6a-dihydro-11-hydroxy-3,3'-dioxo-

CAS Registry Number 145103-60-2

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula C₂₉H₁₆O₇

Molecular Weight 476.43

pH Range 6.0–9.0

Color Change at pH Weak red fluorescence (6.0) to strong red fluorescence (9.0)

pKa 7.6

Physical Form Solid

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide

UV-Visible (λ_{max}) 512 nm, 598 nm

Melting Point >250°C

Boiling Point (Calcd.) 845.9 ± 65.0°C Pressure: 760 Torr

Synthesis Synthetic method¹

Major Applications Sensors,^{2–5} organic electroluminescence (OEL)-based biochips,^{6,7} method for detecting fluorescent molecule,⁸ fluorescence studies of protein crystal nucleation⁹

Safety/Toxicity No data available

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6-CARBOXYNAPHTHOFLOURESCIN

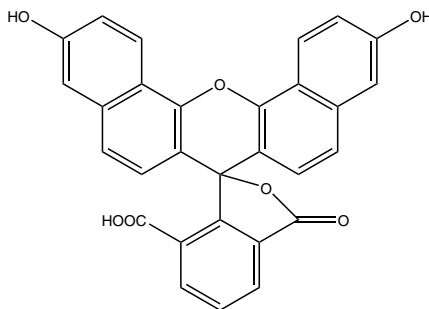
Other Names 6-Carboxynaphthofluorescein

CA Index Name Spiro[7H-dibenzo[c,h]xanthene-7,1'(3'H)-isobenzofuran]-4'-carboxylic acid, 3,11-dihydro-3'-oxo-

CAS Registry Number 145103-61-3

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula $C_{29}H_{16}O_7$

Molecular Weight 476.43

pH Range 6.0–9.0

Color Change at pH Weak red fluorescence (6.0) to strong red fluorescence (9.0)

pKa 7.6

Physical Form Solid

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide

UV-Visible (λ_{max}) 512 nm, 598 nm

Melting Point >250°C

Boiling Point (Calcd.) $851.4 \pm 65.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic method¹

Major Applications Sensors,^{2–5} organic electroluminescence (OEL)-based biochips,^{6,7} fluorescence studies of protein crystal nucleation⁸

Safety/Toxicity No data available

References

1. Wolfbeis, O. S.; Rodriguez, N. V.; Werner, T. LED-compatible fluorosensor for measurement of near-neutral pH values. *Mikrochim. Acta* **1992**, *108*, 133–141.
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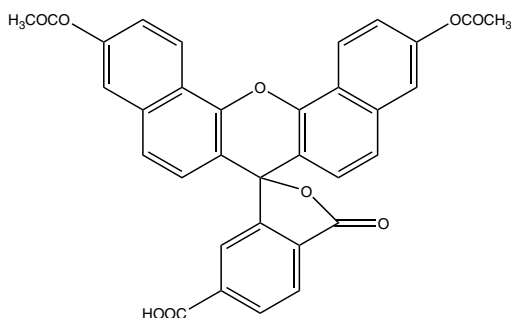
5-CARBOXYNAPHTHOFLUORESCEIN DIACETATE

Other Names 5-Carboxynaphthofluorescein diacetate

CA Index Name Spiro[7H-dibenzo[c,h]xanthene-7,1'(3'H)-isobenzofuran]-5'-carboxylic acid, 3,11-bis(acetyloxy)-3'-oxo-

CAS Registry Number 164256-07-9

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula C₃₃H₂₀O₉

Molecular Weight 560.51

pH Range 6.0–9.0

Color Change at pH Weak red fluorescence (6.0) to strong red fluorescence (9.0)

pKa 7.6

Physical Form Solid

Solubility Insoluble in water; soluble in dimethyl sulfoxide

UV-Visible (λ_{max}) <300 nm

Melting Point >250°C

Boiling Point (Calcd.) 828.4 ± 65.0°C Pressure: 760 Torr

Synthesis Synthetic method¹

Major Applications Sensors¹

Safety/Toxicity No data available

Reference

1. Bentsen, J. G.; Wood, K. B. Sensor with improved drift stability. US Patent 5403746, 1995; *Chem. Abstr.* **1995**, 123, 73757.

CARBOXY SNAFL 1

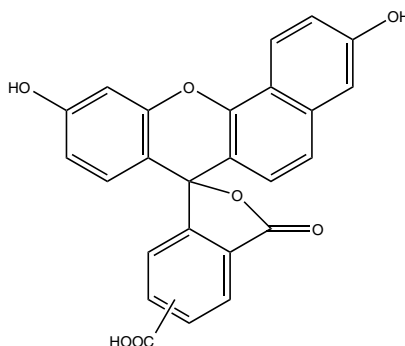
Other Names Carboxy SNAFL 1

CA Index Name Spiro[7H-benzo[c]xanthene-7,1'(3'H)-isobenzofuran]-ar'-carboxylic acid, 3, 10-dihydroxy-3'-oxo-

CAS Registry Number 134344-20-0

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula C₂₅H₁₄O₇

Molecular Weight 426.38

pH Range 6.0–9.0

Color Change at pH Weak green fluorescence (6.0) to strong green fluorescence (9.0)

pKa 7.8

Physical Form Solid

Solubility Soluble in water

UV-Visible (λ_{max}) 508 nm

Melting Point >250°C

Synthesis Synthetic method¹

Major Applications pH Sensors,¹ optical chemical sensors,² biochemical sensors,³ biosensors,⁴ fluorescent pH detector system,⁵ measuring fluorescence lifetime in cells,⁶ determining concentration of a laminar sample stream,⁷ fluorescent reporter beads for fluid analysis,⁸ measuring chemical analytes,⁹ intracellular pH in human sperms,¹⁰ multidrug resistance,¹¹ recording intramitochondrial pH,¹² fluorescent probes¹³

Safety/Toxicity Toxicity in root phloem¹⁴

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CARBOXY SNAFL 2

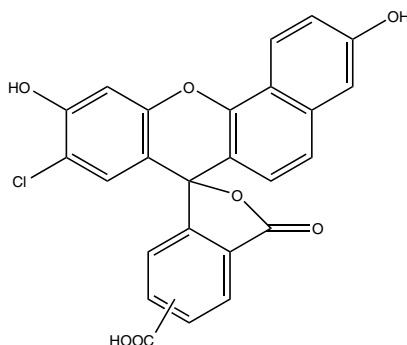
Other Names 10H-Benzo[c]xanthene, benzenedicarboxylic acid derivative; Carboxy-SNAFL 2

CA Index Name Benzenedicarboxylic acid, (9-chloro-3-hydroxy-10-oxo-10H-benzo[c]xanthen-7-yl)-

CAS Registry Number 146472-79-9

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula $C_{25}H_{13}ClO_7$

Molecular Weight 460.83

pH Range 6.0–9.0

Color Change at pH Weak green fluorescence (6.0) to strong green fluorescence (9.0)

pKa 7.7

Physical Form Solid

Solubility Soluble in water

UV-Visible (λ_{max}) 514 nm

Melting Point >250°C

Synthesis Synthetic method¹

Major Applications Sensors,² measuring chemical analytes,³ fluorescence lifetime in cells,⁴ fluorescent pH detector system⁵

Safety/Toxicity No data available

References

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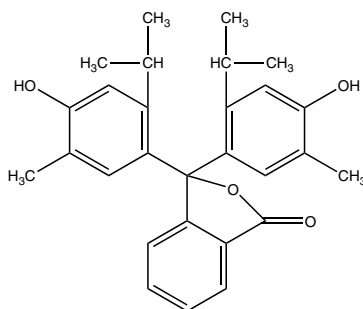
CARVACROLPHTHALEIN

Other Names Phenolphthalein, 2',2''-diisopropyl-5',5''-dimethyl-;

CA Index Name 1(3H)-Isobenzofuranone, 3,3-bis[4-hydroxy-5-methyl-2-(1-methylethyl)phenyl]-

CAS Registry Number 6869-00-7

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Phthalein

Molecular Formula C₂₈H₃₀O₄

Molecular Weight 430.54

pH Range 9.5–10.0

Color Change at pH Colorless (9.5) to blue (10.0)

pKa 9.69

Physical Form Colorless crystals

Solubility Almost insoluble in water; soluble in ethanol

Melting Point 294°C

Boiling Point (Calcd.) 598.9 ± 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Laxatives^{3,4}

Safety/Toxicity No data available

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CHLOROPHENOL RED

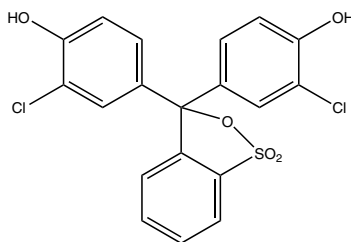
Other Names Chlorophenol red; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-chloro-, S,S-dioxide; *o*-Toluenesulfonic acid, α,α -bis(3-chloro-4-hydroxyphenyl)- α -hydroxy-, γ -sultone; 3H-2,1-Benzoxathiole, phenol derivative; Chlorphenol red; Chlorphenolsulfonphthalein; Dichlorophenolsulfonephthalein; NSC 7828

CA Index Name: Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2-chloro-

CAS Registry Number 4430-20-0

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula $C_{19}H_{12}Cl_2O_5S$

Molecular Weight 423.27

pH Range 4.8–6.4

Color Change at pH Yellow (4.8) to red (6.4)

pKa 6.0

Physical Form Brownish-red or brownish-green powder

Solubility Sparingly soluble in water; soluble in ethanol

UV-Visible (λ_{max}) 572 nm

Melting Point 261–262°C

Boiling Point (Calcd.) $583.0 \pm 50.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods^{1–5}

Major Applications Waveguide,⁶ sol-gel matrix,⁷ display device,⁸ tin electroplating process,⁹ inks,¹⁰ lubricants,¹¹ detergents,¹² preservation of cut flowers,¹³ cosmetics,¹⁴ identifying fresh and stale rice,¹⁵ determining acidity in wine,¹⁶ food storage,¹⁷ detecting lactic acid bacteria,¹⁸ enzyme assays,¹⁹ diagnosis of bacterial and fungal infection,²⁰ oral hygiene products²¹

Safety/Toxicity Oestrogenic activity²²

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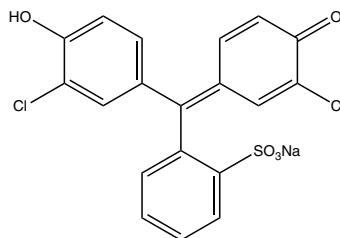
CHLOROPHENOL RED, SODIUM SALT

Other Names Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)*bis*[2-chloro-, *S,S*-dioxide, monosodium salt; Chlorophenol red, sodium salt

CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)*bis*[2-chloro-, monosodium salt

CAS Registry Number 123333-64-2

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Sulfonephthalein

Molecular Formula C₁₉H₁₁Cl₂O₅SNa

Molecular Weight 445.26

pH Range 4.8–6.4

Color Change at pH Yellow (4.8) to red (6.4)

pKa 6.0

Physical Form Brown crystals

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 575 nm

Melting Point >250°C

Synthesis Synthetic methods^{1,2}

Major Applications Aerogel materials,¹ photoreceptors²

Safety/Toxicity No data available

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CHROME ORANGE GR

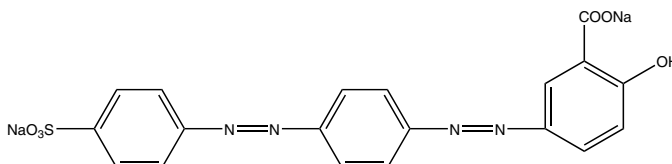
Other Names C.I. Mordant Orange 6; C.I. Mordant Orange 6, disodium salt; Salicylic acid, 5-[*p*-(*p*-sulfophenylazo)phenylazo]-, disodium salt; Acid Chrome Orange GR; Acid Leather Orange CG; Alizarine Chrome Orange GR; Anthracene Orange G; Anthranol Chrome Orange GR; Atlantichrome Orange G; Azochromol Orange AS; Belachrome Fast Orange GR; Brilliant Orange; Brilliant Orange (indicator); C.I. 26520; C.I. Mordant Orange 44; Calcochrome Orange GR; Chromaven Milling Orange G; Chrome Fast Orange G; Chrome Fast Orange GR; Chrome orange; Chrome orange (Russian); Chromocard Orange 3R; Cromal Orange G; Cromal Orange P; Diacromo Orange GR; Diamond Chrome Orange GR; Durochrome Orange G; Eriochrome Orange G; Eriochrome Orange R; Hispacrom Fast Orange GR; Java Chrome Orange EN; Java Unichrome Orange E; Magracrom Orange GR; Mitsui Chrome Orange GR; Monochrome Brilliant Orange GR; Monochrome Orange GR; Naphthalene Leather Yellow R; Neutral Fast Orange G; Omega Chrome Orange G; Solochrome Leather Orange GR; Solochrome Orange GR; Solochrome Orange RS; Sunchromine Orange GR; Synchromate Orange G; Telon Chrome Orange G; Tetrochrome Orange GR; Wool Fast Orange GA-CF; Yodochrome Fast Orange GR

CA Index Name Benzoic acid, 2-hydroxy-5-[[4-[(4-sulfophenyl)azo]phenyl]azo]-, disodium salt

CAS Registry Number 3564-27-0

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula $\text{C}_{19}\text{H}_{12}\text{N}_4\text{O}_6\text{SNa}_2$

Molecular Weight 470.38

pH Range 10.5–12.0

Color Change at pH Yellow (10.5) to red (12.0)

pKa 11.49, 11.71

Physical Form Orange powder

Solubility Soluble in water; very slightly soluble in ethanol, acetone

UV-Visible (λ_{max}) 381 nm

Melting Point $>300^\circ\text{C}$

Synthesis Synthetic method^{1,2}

Major Applications Wool dyeing,^{3–5} soy sauce,⁶ antiAIDS agents⁷

Safety/Toxicity No data available

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CHRYSOIDIN

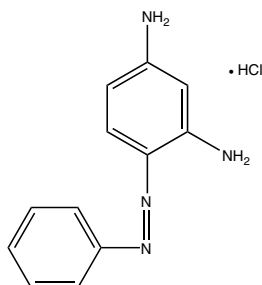
Other Names C.I. Basic Orange 2; C.I. Basic Orange 2, monohydrochloride; 2,4-Diaminoazobenzene hydrochloride; Astra Chrysoidine R; Atlantic Chrysoidine Y; Basic Orange 2; Basonyl Orange 200; Brasilazina Orange Y; C.I. 11270; Calcozine Orange YS; Chrysoidin; Chrysoidin FB; Chrysoidine; Chrysoidine A; Chrysoidine B; Chrysoidine C; Chrysoidine G; Chrysoidine GN; Chrysoidine GS; Chrysoidine HR; Chrysoidine II; Chrysoidine J; Chrysoidine M; Chrysoidine PRL; Chrysoidine PRR; Chrysoidine SL; Chrysoidine SS; Chrysoidine Y; Chrysoidine Y Crystals; Chrysoidine Y Special; Chrysoidine YL; Chrysoidine YN; Chrysoidine hydrochloride; Chrysoidine orange; Diazocard Chrysoidine G; Leather Orange HR; Nippon Kagaku Chrysoidine; Pure Chrysoidine YBH; Sugai Chrysoidine; Tertrophene Brown CG; Verona Chrysoidine GN

CA Index Name 1,3-Benzenediamine, 4-(phenylazo)-, monohydrochloride

CAS Registry Number 532-82-1

Merck Index Number 2257

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula C₁₂H₁₂N₄·HCl

Molecular Weight 248.72

pH Range 4.0–7.0

Color Change at pH Orange (4.0) to yellow (7.0)

Physical Form Reddish-brown crystals

Solubility Soluble in water, ethanol, acetone, methyl cellosolve, xylene; practically insoluble in benzene

UV-Visible (λ_{max}) 449 nm

Melting Point 118–118.5°C

Boiling Point 2262°C

Synthesis Synthetic methods^{1–4}

Major Applications Recording materials,⁵ waveguides,⁶ thin solid films,⁷ photographic materials,⁸ printing plates,⁹ inks,^{10–12} toners,¹³ detergents,¹⁴ corrosion inhibitors,¹⁵ rubber,¹⁶ textiles,^{17–19} hair dyes²⁰

Safety/Toxicity Toxicological evaluation,²¹ mutagenicity,²² carcinogenicity²³

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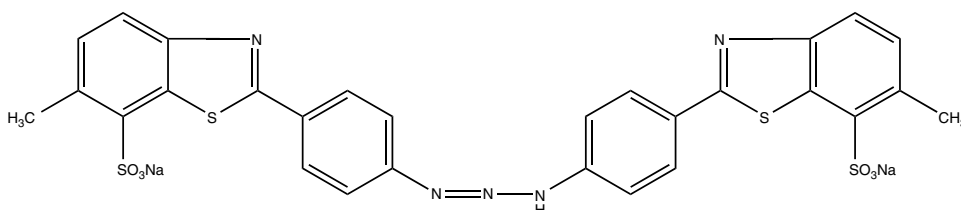
CLAYTON YELLOW

Other Names C.I. Direct Yellow 9; C.I. Direct Yellow 9, disodium salt; Clayton Yellow; Atlantic Brilliant Yellow MN; Benzo Yellow TZ; C.I. 19540; Chlorazol Yellow 2G; Chlorazol Yellow DP; Diaphtamine Brilliant Yellow 6GS; Diazamine Golden Yellow T; Diazol Yellow J; Direct Yellow MTZ; Direct Yellow TZ; Ferro 42-145A; Hispamin Pure Yellow T2G; Mimosa Z; Peeramine Bright Yellow MN; Pontamine Pure Yellow; Pontamine Pure Yellow MN; Thiazol Yellow; Thiazol Yellow G; Thiazol Yellow GGM; Thiazol Yellow R; Thiazol Yellow Z; Thiazole Y; Thiazole Yellow G; Thiazole Yellow GGM; Thiazole yellow; Titan Yellow; Titan Yellow Dye; Titan Yellow G

CA Index Name 7-Benzothiazolesulfonic acid, 2,2'-(1-triazene-1,3-diyl-di-4,1-phenylene)bis[6-methyl-, disodium salt

CAS Registry Number 1829-00-1

Merck Index Number 9310

Chemical Structure

Chemical/Dye Class Azo, thiazole

Molecular Formula $C_{28}H_{19}N_5O_6S_4Na_2$

Molecular Weight 695.73

pH Range 11.0–13.0

Color Change at pH Yellow (11.0) to red (13.0)

Physical Form Yellowish-brown powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 402 nm

Melting Point >250°C

Synthesis Synthetic methods^{1–4}

Major Applications Display device,⁵ optical sensors,^{6,7} thin-film device,⁸ incandescent electric lamps,⁹ photoreceptors,¹⁰ lithographic process,¹¹ inks,¹² pencil leads,¹³ paints,¹⁴ adhesives,¹⁵ plastic materials,¹⁶ molding materials,¹⁷ steel plates,¹⁸ detection of albumin,¹⁹ treatment of amyloidosis disorders,²⁰ treatment of apolipoprotein E-related diseases²¹

Safety/Toxicity Eye irritation test²²

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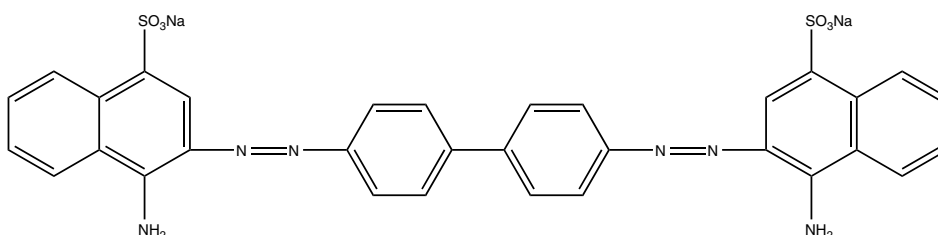
CONGO RED

Other Names C.I. Direct Red 28, disodium salt; Atlantic Congo Red; Atul Congo Red; Azocard Red Congo; Benzo Congo Red; Brasilamina Congo 4B; C.I. 22120; C.I. Direct Red 28; Congo Red 4B; Congo Red 4BX; Congo Red CR; Congo Red H; Congo Red K; Congo Red L; Congo Red M; Congo Red N; Congo Red R; Congo Red RS; Congo Red W; Congo Red WS; Congo Red sodium salt; Congo red; Cotton Red 4BC; Cotton Red 5B; Cotton Red L; Diacotton Congo Red; Direct Congo Red; Direct Red 28; Direct Red C; Direct Red DC-CF; Direct Red K; Erie Congo 4B; Haemomedical; Haemonorm; Hemorrhagyl; Hispamin Congo 4B; Kayaku Congo Red; Mitsui Congo Red; Peeramine Congo Red; Red K; Solucongo; Sugai Congo Red; Tertrodirect Red C; Trisulfon Congo Red; Vondacel Red CL

CA Index Name 1-Naphthalenesulfonic acid, 3,3'-[[1,1'-biphenyl]-4,4'-diylbis-(azo)]bis[4-amino-, disodium salt

CAS Registry Number 573-58-0

Merck Index Number 2498

Chemical Structure

Chemical/Dye Class Azo

Molecular Formula $C_{32}H_{22}N_6O_6S_2Na_2$

Molecular Weight 696.67

pH Range 3.0–5.0

Color Change at pH Blue (3.0) to red (5.0)

pKa 4.1

Physical Form Brownish-red powder

Solubility Soluble in water, ethanol; very slightly soluble in acetone; practically insoluble in ether, xylene

UV-Visible (λ_{max}) 497 nm, 488 nm, 595 nm

Melting Point $>360^\circ\text{C}$

Synthesis Synthetic methods^{1–9}

Major Applications Waveguides,¹⁰ optical sensors,¹¹ display devices,¹² inks,¹³ fertilizer,¹⁴ pesticides,¹⁵ detecting carbohydrates,¹⁶ treatment of pathogen infections,¹⁷ age-related macular degeneration,¹⁸ amyloid accumulation in the brain¹⁹

Safety/Toxicity Acute toxicity,²⁰ carcinogenicity,²¹ cutaneous toxicity,²² cytotoxicity,²³ genotoxicity,²⁴ mutagenicity,²⁵ neurotoxicity²⁶

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COUMARIN

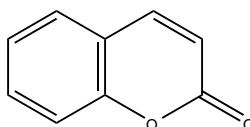
Other Names Coumarin; 1,2-Benzopyrone; 2-Propenoic acid, 3-(2-hydroxyphenyl)-, δ -lactone; 5,6-Benzo-2-pyrone; Benzo- α -pyrone; Coumarinic anhydride; NSC 8774; Rattex; Tonka bean camphor; cis-*o*-Coumarinic acid lactone; *o*-Hydroxycinnamic acid lactone

CA Index Name 2H-1-Benzopyran-2-one

CAS Registry Number 91-64-5

Merck Index Number 2562

Chemical Structure



C

Chemical/Dye Class Fluorescent, Coumarin

Molecular Formula $C_9H_6O_2$

Molecular Weight 146.14

pH Range 9.5–10.5

Color Change at pH Nonfluorescence (9.5) to light green fluorescence (10.5)

Physical Form White powder

Solubility Very slightly soluble in water; freely soluble in ethanol, ether, chloroform

UV-Visible (λ_{max}) 275 nm

Melting Point 68–70°C

Boiling Point 297–299°C

Synthesis Synthetic methods^{1–14}

Major Applications Color filter,¹⁵ organic electroluminescent devices,^{15,16} liquid crystal displays,¹⁷ field emission displays,¹⁸ inks,¹⁹ nickel plating,²⁰ detergents,²¹ deodorant for shoes,²² petroleum products,²³ cigarettes,²⁴ personal care products,²⁵ cosmetics,²⁶ sunscreen cream,²⁷ perfumes,²⁸ enzyme substrates,²⁹ nucleic acid sequencing,³⁰ antiinflammatory agent,³¹ treatment of cancer,³² neurotransmission disorders,³³ bleeding disorders,³⁴ cerebrovascular disease,³⁵ thrombosis,³⁶ hemorrhoids,³⁷ rheumatic disease,³⁸ arthritic disease,³⁸ epilepsy,³⁹ vaginitis,⁴⁰ painkiller,⁴¹ teeth whitening agent,⁴² skin whitening agent,⁴³ wound healing promoter⁴⁴

Safety/Toxicity Carcinogenicity,⁴⁵ cell toxicity,⁴⁶ ecotoxicity,⁴⁷ effects on breast feeding,⁴⁸ effects on children during pregnancy,⁴⁹ genotoxicity,⁵⁰ hepatotoxicity,⁵¹ in vitro toxicity,⁵² mutagenicity,⁵³ neurotoxicity⁵⁴

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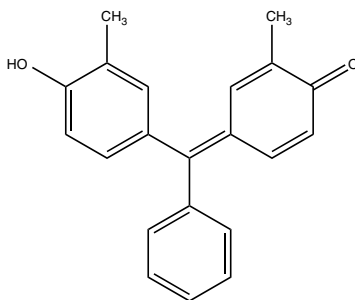
o-CRESOLBENZEIN

Other Names 2,5-Cyclohexadien-1-one, 4-(4-hydroxy-3-methyl- α -phenylbenzylidene)-2-methyl-;
o-Cresolbenzein

CA Index Name 2,5-Cyclohexadien-1-one, 4-[(4-hydroxy-3-methylphenyl)-phenylmethylene]-2-methyl-

CAS Registry Number 5664-07-3

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Benzein

Molecular Formula $C_{21}H_{18}O_2$

Molecular Weight: 302.37

pH Range 7.2–8.6

Color Change at pH Yellow (7.2) to red (8.6)

pKa 9.66

Physical Form Red-orange crystals

Solubility Insoluble in water; soluble in ethanol

Melting Point 260–262°C

Boiling Point (Calcd.) $505.4 \pm 50.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Cosmetics³

Safety/Toxicity No data available

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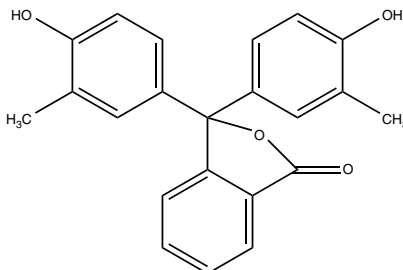
o-CRESOLPHTHALEIN

Other Names Phenolphthalein, 3',3''-dimethyl-; o-Cresolphthalein; 3,3-Bis(3-methyl-4-hydroxyphenyl)phthalide; Cresolphthalein

CA Index Name 1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxy-3-methylphenyl)-

CAS Registry Number 596-27-0

Merck Index Number 2576

Chemical Structure

Chemical/Dye Class Phthalein

Molecular Formula C₂₂H₁₈O₄

Molecular Weight 346.38

pH Range 8.2–9.8

Color Change at pH Colorless (8.2) to red (9.8)

pKa 9.40

Physical Form Buff or beige powder

Solubility Slightly soluble in water; soluble in ethanol

UV-Visible (λ_{max}) 566 nm, 381 nm

Melting Point 223°C

Boiling Point (Calcd.) 555.0 ± 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–8}

Major Applications Sensors,^{9–11} display device,¹² photoresists,¹³ recording materials,¹⁴ imaging materials,¹⁵ authentication system for secure documents,¹⁶ decoder system,¹⁷ lithium cells,¹⁸ electroplating process,¹⁹ inks,^{20,21} markers,²² toners,²³ correction fluid,²⁴ paints,²⁵ adhesives,^{26,27} floor coatings,²⁸ gas leaking detector for safety in industries,²⁹ toys,³⁰ food storage,³¹ diapers,³² determination of calcium,³³ lotions,³⁴ urine analysis test strips,³⁵ drugs,³⁶ blood analysis³⁷

Safety/Toxicity Toxic effects to health and environments³⁸

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o-CRESOLPHTHALEIN COMPLEXON

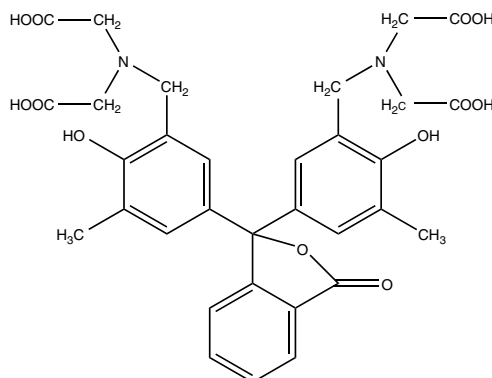
Other Names Phenolphthalein, 3',3''-bis[[bis(carboxymethyl)amino]methyl]-5',5''-dimethyl-; 3,3'-Bis[*N,N*-bis(carboxymethyl)aminomethyl]-*o*-cresolphthalein; 3,3'-Bis[*N,N*-di(carboxymethyl)aminomethyl]-*o*-cresolphthalein; Cresolphthalein complexon; Cresolphthalexon; NSC 298195; Phthalein complexone; *o*-Cresolphthalein complexon; *o*-Cresolphthalein complexone; *o*-Cresolphthalexon; *o*-Cresolphthalexone; Metalphthalein; Phthalein Purple

CA Index Name Glycine, *N,N'*-[(3-oxo-1(3H)-isobenzofuranylidene)bis[(6-hydroxy-5-methyl-3,1-phenylene)methylene]]bis[*N*-(carboxymethyl)-

CAS Registry Number 2411-89-4

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Phthalein

Molecular Formula C₃₂H₃₂N₂O₁₂

Molecular Weight 636.60

pH Range 8.2–9.8

Color Change at pH Colorless (8.2) to red (9.8)

pKa 1.47, 8.24

Physical Form Light pink powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 575 nm, 377 nm

Melting Point 181–185°C

Boiling Point (Calcd.) 892.1 ± 65.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–6}

Major Applications Sensors,^{7–10} photoconductors,¹¹ copying materials,¹² rubber,^{13–15} body fluid testing,¹⁶ determination of calcium,¹⁷ magnesium,¹⁸ tin,¹⁹ method for measuring urea nitrogen,²⁰ liposomal construct for diagnostic use,²¹ cardiovascular disease,²² antibacterial agent²³

Safety/Toxicity *In vitro* toxicity²³

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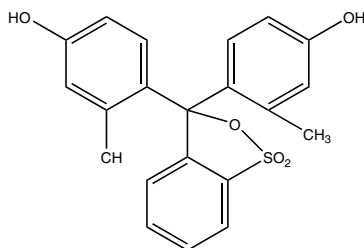
***m*-CRESOL PURPLE**

Other Names Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[3-methyl-, *S,S*-dioxide; *m*-Cresol purple; *m*-Cresol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)di-, *S,S*-dioxide; *o*-Toluenesulfonic acid, α -hydroxy- α,α -bis(4-hydroxy-*o*-tolyl)-, γ -sultone; 3H-2,1-Benzoxathiole, phenol derivative; Cresol purple; Metacresol Purple; NSC 9607; *m*-Cresolsulfonephthalein

CA Index Name: Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[3-methyl-

CAS Registry Number: 2303-01-7

Merck Index Number 2577

Chemical Structure

Chemical/Dye Class: Sulfonephthalein

Molecular Formula: C₂₁H₁₈O₅S

Molecular Weight: 382.43

pH Range 1.2–2.8;

7.4–9.0

Color Change at pH Red (1.2) to yellow (2.8)

Yellow (7.4) to purple (9.0)

pKa 1.51, 8.32

Physical Form Dark brown glittering crystals or olive green powder

Solubility Very slightly soluble in water, ethanol; soluble in methanol

UV-Visible (λ_{max}) 579 nm, 371 nm

Melting Point >250°C

Boiling Point (Calcd.) 577.5 $\pm$ 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–5}

Major Applications Fuel cells,⁶ sensors,⁷ display device,⁸ falsification-proof security paper,⁹ inks,¹⁰ correction fluid,¹¹ paints,¹² detection of electrophilic gases,¹³ lubricants,¹⁴ cement products,¹⁵ packaging system,¹⁶ adhesive,¹⁷ cosmetics,¹⁸ food storage,¹⁹ determining glucose in dialysis solution,²⁰ screening of cat diseases,²¹ detecting carbohydrates,²² oral hygiene products²³

Safety/Toxicity No data available

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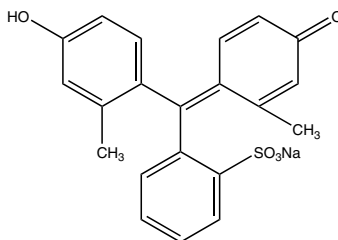
m-CRESOL PURPLE, SODIUM SALT

Other Names Phenol, 4,4'-(3H-1,2-benzoxathiol-3-ylidene)bis[3-methyl-, S,S-dioxide, monosodium salt; 3H-1,2-Benzoxathiole, phenol derivative

CA Index Name Phenol, 4,4'-(2,2-dioxido-3H-1,2-benzoxathiol-3-ylidene)bis[3-methyl-, monosodium salt

CAS Registry Number 62625-31-4

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class: Sulfonephthalein

Molecular Formula C₂₁H₁₇O₅SNa

Molecular Weight 404.42

pH Range 1.2–2.8

7.4–9.0

Color Change at pH Red (1.2) to yellow (2.8)

Yellow (7.4) to purple (9.0)

pKa 1.51, 8.32

Physical Form Black powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 436 nm

Melting Point >250°C

Synthesis Synthetic method¹

Major Applications Screening method of endocrine disrupting chemicals²

Safety/Toxicity No data available

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o-CRESOL RED

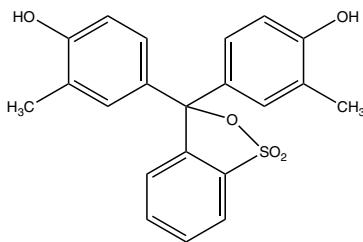
Other Names Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-methyl-, S,S-dioxide; o-Cresol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)di-, S,S-dioxide; o-Cresolsulfonephthalein; o-Toluenesulfonic acid, α -hydroxy- α,α -bis(4-hydroxy-*m*-tolyl)-, γ -sultone; 3H-2,1-Benzoxathiole, phenol derivative; 3',3''-Dimethylphenolsulfonephthalein; Cresol red; Cresolsulfophthalein; NSC 7224; o-Cresol Red; o-Cresolsulfonphthalein

CA Index Name: Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2-methyl-

CAS Registry Number: 1733-12-6

Merck Index Number 2578

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula C₂₁H₁₈O₅S

Molecular Weight 382.43

pH Range 0.2–1.8

7.0–8.8

Color Change at pH Red (0.2) to yellow (1.8)

Yellow (7.0) to reddish-purple (8.8)

pKa 1.4, 8.2, 8.3

Physical Form Green glittering crystals or reddish-brown powder

Solubility Sparingly soluble in water; soluble in ethanol

UV-Visible (λ_{max}) 570 nm, 367 nm, 432 nm

Melting Point >300°C

Boiling Point (Calcd.) 561.9 $\pm$ 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–5}

Major Applications Display device,⁶ optical sensors,⁷ combustion gas detection system,⁸ inks,⁹ correction fluid,¹⁰ diapers,¹¹ toothpaste,¹² identifying fresh and stale rice,¹³ food storage,¹⁴ determine glucose in dialysis solution,¹⁵ monitor metabolic activity of microorganisms,¹⁶ detect bacterial infection,¹⁷ psychoactive drugs,¹⁸ dental impression material¹⁹

Safety/Toxicity No data available

References

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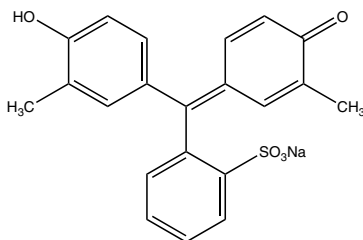
o-CRESOL RED, SODIUM SALT

Other Names Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2-methyl-, S,S-dioxide, monosodium salt; 3H-2,1-Benzoxathiole, phenol derivative

CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2-methyl-, monosodium salt

CAS Registry Number 62625-29-0

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Sulfonephthalein

Molecular Formula C₂₁H₁₇O₅SNa

Molecular Weight 404.42

pH Range 0.2–1.8

7.0–8.8

Color Change at pH Red (0.2) to yellow (1.8)

Yellow (7.0) to reddish-purple (8.8)

pKa 1.4, 8.2, 8.3

Physical Form Brown powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 425 nm

Melting Point 250°C (decompose)

Synthesis Synthetic method¹

Major Applications Thermochromic materials,² cosmetics,¹ measurement of hydrophobicity of therapeutic drugs³

Safety/Toxicity No data available

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CRYSTAL VIOLET

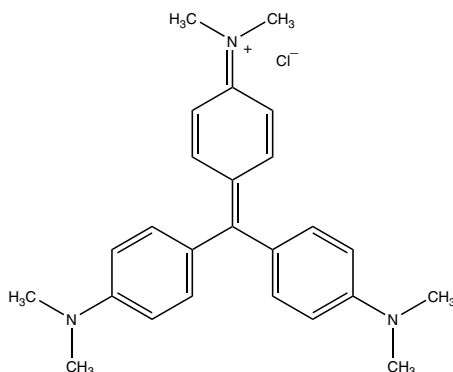
Other Names C.I. Basic Violet 3; 12416 Violet; Adergon; Aizen Crystal Violet; Aizen Crystal Violet Extra Pure; Aniline violet; Aniline violet pyoktanine; Atmonil; Avermin; Axuris; Badil; Basic Violet 3; Basic Violet BN; Basonyl Violet 610; C.I. 42555; Calcozine Violet 6BN; Calcozine Violet C; Crystal Violet 10B; Crystal Violet 5BO; Crystal Violet 6B; Crystal Violet 6BO; Crystal Violet AO; Crystal Violet AON; Crystal Violet BP; Crystal Violet BPC; Crystal Violet Extra Pure; Crystal Violet Extra Pure APN; Crystal Violet Extra Pure APNX; Crystal Violet FN; Crystal Violet HL 2; Crystal Violet O; Crystal Violet Pure DSC; Crystal Violet Pure DSC Brilliant; Crystal Violet SS; Crystal Violet Technical; Crystal Violet USP; Crystal Violet chloride; Crystal violet; Gentersal; Gentian Violet B; Gentian violet; Gentiaverm; Gentacid; Genticioletten; Hecto Violet R; Hectograph Violet SR; Hexamethyl violet; Hexamethyl-*p*-rosaniline chloride; Hexamethylpararosaniline chloride; Hidaco Brilliant Crystal Violet; Meroxyl; Meroxyl-Wander; Meroxylan; Meroxylan-Wander; Methyl Violet 10B; Methyl Violet 10BD; Methyl Violet 10BK; Methyl Violet 10BN; Methyl Violet 10BNS; Methyl Violet 10BO; Methyl Violet 5BNO; Methyl Violet 5BO; Methyl Violet 6B; Methyl Violet 6B (biological stain); Methylrosaniline chloride; Methylrosanilinium chloride; Mitsui Crystal Violet; Oxiuran; Oxycolor; Oxyozyl; Paper Blue R; Pararosaniline, *N,N,N',N',N'',N''*-hexamethyl-, chloride; Plastoresin Violet 5BO; Pyoktanin; Sanyo Fanal Violet R; Vermicid; Vianin; Viocid; Violet 5BO; Violet 6BN; Violet CP; Violet XXIII; crystal violet

CA Index Name Methanaminium, *N*-[4-*bis*[4-(dimethylamino)phenyl]methylene]-2,5-cyclohexadien-1-ylidene]-*N*-methyl-, chloride

CAS Registry Number 548-62-9

Merck Index Number 4395

Chemical Structure



Chemical/Dye Class Triphenylmethane

Molecular Formula $C_{25}H_{30}N_3Cl$

Molecular Weight 407.99

pH Range 0.0–2.0

Color Change at pH Yellow (0.0) to blue-violet (2.0)

pKa 9.4

Physical Form Green to yellowish-green powder

Solubility Soluble in water, acetone, chloroform; very soluble in ethanol; practically insoluble in ether; insoluble in xylene

UV-Visible (λ_{max}) 590 nm

Melting Point 205–215°C (decompose)

Synthesis Synthetic methods^{1–12}

Major Applications Photoresists,¹³ lithographic printing plate,¹⁴ printed circuit board,¹⁵ inks,¹⁶ detergent,¹⁷ hair dyes,¹⁸ shampoo,¹⁹ drug screening method,²⁰ bone cement preparation method,²¹ treating microorganisms,²² hemorrhoids,²³ antifungal,²⁴ antibacterial,²⁵ antimalarial agent,²⁶ dental application²⁷

Safety/Toxicity Acute oral toxicity,²⁸ chronic toxicity,^{29,30} carcinogenicity,^{29,30} cytotoxicity,³¹ genotoxicity,³² mutagenicity,^{33,34} ototoxicity,³⁵ percutaneous toxicity,³⁶ phototoxicity³⁷

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CURCUMIN

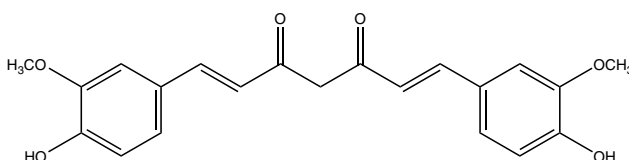
Other Names 1,6-Heptadiene-3,5-dione, 1,7-bis(4-hydroxy-3-methoxyphenyl)-, (E,E)-; Curcumin; (E,E)-1,7-Bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione; C Yellow 15; C.I. 75300; C.I. Natural Yellow 3; Curcuma; Curcumin I; Curcumine; Diferuloylmethane; E 100; E 100 (dye); Haidr; Halad; Haldar; Halud; Indian Saffron; Kacha Haldi; Merita Earth; NSC 32982; Natural Yellow 3; San-Ei Curcumine AL; San-Ei Gen Curcumine AL; Souchet; Terra Merita; Turmeric; Turmeric (dye); Turmeric yellow; Ukon; Ukon (dye); Yellow Ginger; Yellow Root; Yo-Kin; trans,trans-Curcumin

CA Index Name 1,6-Heptadiene-3,5-dione, 1,7-bis(4-hydroxy-3-methoxyphenyl)-, (1E,6E)-

CAS Registry Number 458-37-7

Merck Index Number 2673

Chemical Structure



Chemical/Dye Class Miscellaneous, Chalcone

Molecular Formula C₂₁H₂₀O₆

Molecular Weight 368.38

pH Range 7.8–9.2

Color Change at pH Yellow (7.8) to red-brown (9.2)

pKa 8.09

Physical Form Orange-yellow crystalline powder

Solubility Insoluble in water, ether; soluble in ethanol, acetic acid, dimethyl sulfoxide

UV-Visible (λ_{max}) 430 nm

Melting Point 183°C

Boiling Point (Calcd.) 591.4 ± 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–7}

Major Applications Cosmetics,⁸ drug-eluting stents,⁹ inhibition of formation of skin-wrinkles,¹⁰ treating alzheimer's disease,¹¹ skin diseases,¹² coronary restenosis,¹³ diabetes,¹⁴ obesity,¹⁴ leukemia,¹⁵ neurofibromas,¹⁶ cancer,¹⁷ antimicrobial,¹⁸ antiviral,¹⁹ antiinflammatory,²⁰ antiprostata cancer²¹

Safety/Toxicity Mitochondrial and DNA damage,²² chronic toxicity,²³ tissue-specific toxicity,²⁴ carcinogenicity,^{25,26} cytotoxicity,²⁷ excitotoxicity,²⁸ hepatotoxicity,²⁹ oral toxicity,³⁰ mutagenicity³¹

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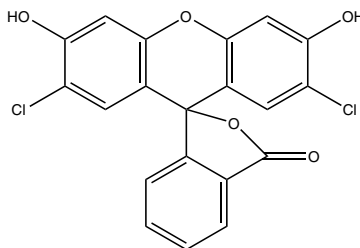
Other Names Fluorescein, 2',7'-dichloro-; 2',7'-Dichlorofluorescein; D and C Orange 25; D and C Orange No. 25; Fluorescein 27; Fluorescein 548

CA Index Name Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 2',7'-dichloro-3',6'-dihydroxy-

CAS Registry Number 76-54-0

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula C₂₀H₁₀Cl₂O₅

Molecular Weight 401.20

pH Range 4.0–6.0

Color Change at pH Weak green fluorescence (4.0) to intense green fluorescence (6.0)

pKa 4.46

Physical Form Light orange powder

Solubility Insoluble in water; soluble in ethanol; slightly soluble in ether, methanol

UV-Visible (λ_{max}) 509 nm

Melting Point >250°C

Boiling Point (Calcd.) 634.4 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Electroluminescent devices,³ sol-gel silica films,⁴ integrated circuits,⁵ photoresists,⁶ recording material,⁷ LED devices,⁸ photoconductors,⁹ Solid-state dye laser,¹⁰ lithographic printing plates,¹¹ inks,¹² Fluorescent pH sensors,¹³ emissive probes,¹⁴ chemotherapeutic treatment of disease,¹⁵ phototherapeutic treatment of disease,¹⁶ photodynamic treatment of disease¹⁷

Safety/Toxicity Carcinogenicity,¹⁸ cytotoxicity,¹⁹ genotoxicity,²⁰ hemoglobin toxicity,²¹ neurotoxicity,²² phototoxicity.²³

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6,7-DIHYDROXYCOUMARIN

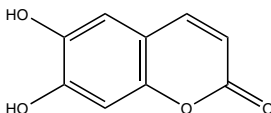
Other Names Coumarin, 6,7-dihydroxy-; Esculetin; 6,7-Dihydroxy-2-benzopyrone; 6,7-Dihydroxycoumarin; Aesculetin; Asculetine; Cichorigenin; Cichoriin aglycon; Esculetol; Esculin aglycon; NSC 26428; Esculetin

CA Index Name 2H-1-Benzopyran-2-one, 6,7-dihydroxy-

CAS Registry Number 305-01-1

Merck Index Number 3697

Chemical Structure



Chemical/Dye Class Fluorescent, Coumarin

Molecular Formula C₉H₆O₄

Molecular Weight 178.14

pH Range 1.5–2.0

Color Change at pH Weak blue fluorescence (1.5) to strong blue fluorescence (2.0)

pKa 1.71

Physical Form Light yellow powder

Solubility Almost insoluble in boiling water, ether; soluble in hot ethanol, glacial acetic acid

Melting Point 272–274°C

Boiling Point (Calcd.) 469.7 ± 45.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–10}

Major Applications Herbicides,¹¹ cosmetics,¹² teeth whitening agent,¹³ antiinflammatory,¹⁴ antifungal,¹⁵ antibacterial,¹⁵ antiviral,¹⁶ treating drug-induced weight gain,¹⁷ neurodegenerative and blood coagulation disorders,¹⁸ cancer,¹⁹ amyloidosis,²⁰ skin impairments and baldness²¹

Safety/Toxicity Cytotoxicity,²² mutagenicity²³

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3,6-DIHYDROXYPHTHALIMIDE

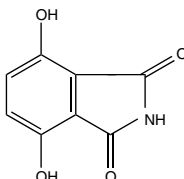
Other Names Phthalimide, 3,6-dihydroxy-; 3,6-Dihydroxyphthalimide; NSC 229301

CA Index Name 1H-Isoindole-1,3(2H)-dione, 4,7-dihydroxy-

CAS Registry Number 51674-11-4

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula C₈H₅NO₄

Molecular Weight 179.13

pH Range 0.0–2.4;

6.0–8.0

Color Change at pH Blue fluorescence (0.0) to green fluorescence (2.4)

Green fluorescence (6.0) to yellow/green fluorescence (8.0)

pKa 1.65, 6.97

Physical Form White solid

Solubility Insoluble in water; soluble in ethanol, methanol

Melting Point >250°C

Synthesis Synthetic methods^{1–4}

Major Applications Dye lasers,⁵ immunomodulatory assays⁶

Safety/Toxicity No data available

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4-DIMETHYLAMINO-2-METHYLAZOBENZENE

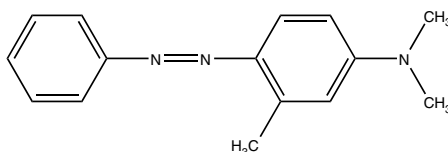
Other Names *m*-Toluidine, *N,N*-dimethyl-4-(phenylazo)-; 2-MeDAB; 2-Methyl-4-(dimethylamino) azobenzene; 4-(Dimethylamino)-2-methylazobenzene; 4-(*N,N*-Dimethylamino)-2-methylazobenzene; *N,N*-Dimethyl-4-(phenylazo)-*m*-toluidine; NSC 102372

CA Index Name Benzenamine, *N,N*,3-trimethyl-4-(phenylazo)-

CAS Registry Number 54-88-6

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula C₁₅H₁₇N₃

Molecular Weight 239.32

pH Range 2.8–4.4

Color Change at pH Red (2.8) to yellow (4.4)

pKa 3.68

Physical Form Red-orange crystals

Solubility Practically insoluble in water; soluble in ethanol, acetone

UV-Visible (λ_{max}) 420 nm

Melting Point 67–69°C

Boiling Point (Calcd.) 390.9 ± 35.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Nematocides,^{3,4} as diagnostic agent for diseases related with amyloid accumulation,⁵ hepatocarcinogenesis⁶

Safety/Toxicity Carcinogenicity,^{7–13} mutagenicity,^{14–22} chromosome aberration,²³ cytotoxicity²⁴

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DINITROCRESOL

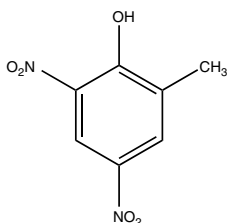
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CA Index Name Phenol, 2-methyl-4,6-dinitro-

CAS Registry Number 534-52-1

Merck Index Number 3279

Chemical Structure



Chemical/Dye Class Nitro

Molecular Formula $C_7H_6N_2O_5$

Molecular Weight 198.13

pH Range 2.4–3.8

Color Change at pH Colorless (2.4) to yellow (3.8)

pKa 4.42

Physical Form Yellow prisms

Solubility Sparingly soluble in water; readily soluble in ethanol, acetone, ether

Melting Point 87.5°C

Boiling Point 378°C

Synthesis Synthetic methods^{1–8}

Major Applications Explosives,⁹ fungicides,¹⁰ herbicides,^{11,12} insecticides,^{13,14} pesticides,^{15,16} anti-tumor agent,¹⁷

Safety/Toxicity Acute toxicity,¹⁸ aquatic toxicity,¹⁹ ecotoxicity,²⁰ environmental pollutants,²¹ mutagenicity,²² spermatotoxic effects²³

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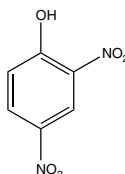
α -DINITROPHENOL

Other Names α -Dinitrophenol; 1-Hydroxy-2,4-dinitrobenzene; 2,4-DNP; 2,4-Dinitrophenol; Aldifen; DNP; Dinitrophenol; Dinofan; Fenoxyl Carbon N; NSC 1532; Nitrophen; Nitrophen; Phenol, α -dinitro-

CA Index Name Phenol, 2,4-dinitro-

CAS Registry Number 51-28-5

Merck Index Number 3280

Chemical Structure

Chemical/Dye Class Nitro

Molecular Formula $C_6H_4N_2O_5$

Molecular Weight 184.11

pH Range 2.0–4.7

Color Change at pH Colorless (2.0) to yellow (4.7)

pKa 3.8, 3.9, 4.0, 4.1

Physical Form Light yellow crystals

Solubility Sparingly soluble in water; soluble in ethanol, benzene

Melting Point 112–114°C

Boiling Point (Calcd.) $312.1 \pm 27.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods^{1–10}

Major Applications Display device,¹¹ recording materials,¹² inks,¹³ paints,¹⁴ method for preserving food,¹⁵ method for gene expression profiling,¹⁶ treatment of parasitic diseases,¹⁷ neurological diseases,¹⁸ epilepsy,¹⁹ cancer,^{20–22} keratin materials,²³ neoplasms,²⁴ infectious diseases,²⁵ neutropenia,²⁶ detecting chromosome aberrations,²⁷ bacteria in gastrointestinal track²⁸

Safety/Toxicity Acute toxicity,²⁹ ecotoxicity,³⁰ cytotoxicity,³¹ environmental toxicity,³² genotoxicity³³

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β -DINITROPHENOL

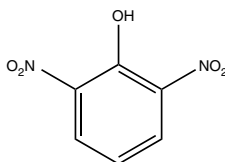
Other Names β -Dinitrophenol; 2,6-DNP; 2,6-Dinitrophenol; NSC 6215; Phenol, β -dinitro-; *o*-Dinitrophenol

CA Index Name Phenol, 2,6-dinitro-

CAS Registry Number 573-56-8

Merck Index Number 3282

Chemical Structure



Chemical/Dye Class Nitro

Molecular Formula $C_6H_4N_2O_5$

Molecular Weight 184.11

pH Range 1.7–4.4

Color Change at pH Colorless (1.7) to yellow (4.4)

pKa 3.69, 3.7, 3.5

Physical Form Yellowish crystals

Solubility Sparingly soluble in water; soluble in ethanol, chloroform, ether

Melting Point 63–64°C

Boiling Point (Calcd.) 239.0 $\pm$ 20.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–7}

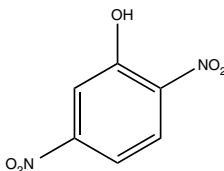
Major Applications Energetic materials,⁸ battery,⁹ lubricants,¹⁰ curing agents for epoxy resins,¹¹ fungicidal,¹² herbicidal,¹³ food storage,¹⁴ drugs¹⁵

Safety/Toxicity Ecotoxicity,¹⁶ acute toxicity,¹⁷ mutagenicity¹⁸

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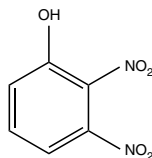
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γ -DINITROPHENOL**Other Name** 2,5-DNP; 2,5-Dinitrophenol; NSC 90441; Phenol, γ -dinitro-**CA Index Name** Phenol, 2,5-dinitro-**CAS Registry Number** 329-71-5**Merck Index Number** 3281**Chemical Structure****D****Chemical/Dye Class** Nitro**Molecular Formula** $C_6H_4N_2O_5$ **Molecular Weight** 184.11**pH Range** 4.0–5.8**Color Change at pH** Colorless (4.0) to yellow (5.8)**pKa** 5.21, 5.1, 5.0**Physical Form** Yellowish needles**Solubility** Sparingly soluble in water; soluble in ethanol, ether**Melting Point** 108°C**Boiling Point (Calcd.)** $309.6 \pm 27.0^\circ\text{C}$ Pressure: 760 Torr**Synthesis** Synthetic methods^{1–6}**Major Applications** Liquid crystal films,⁷ electrophotographic materials,⁸ adhesives,⁹ inks,¹⁰ lubricants,¹¹ preservation of cut flowers,^{12,13} food storage,¹⁴ materials for evaluating dental caries activity¹⁵**Safety/Toxicity** Aquatic toxicity,¹⁶ cytotoxicity,¹⁷ ecotoxicity,¹⁸ environmental toxicity¹⁹**References**

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ϵ -DINITROPHENOL**Other Names** 2,3-DNP; 2,3-Dinitrophenol; NSC 156083**CA Index Name** Phenol, 2,3-dinitro-**CAS Registry Number** 66-56-8**Merck Index Number** Not listed**Chemical Structur****D****Chemical/Dye Class** Nitro**Molecular Formula** $C_6H_4N_2O_5$ **Molecular Weight** 184.11**pH Range** 3.9–5.9**Color Change at pH** Colorless (3.9) to yellow (5.9)**pKa** 4.86, 4.96**Physical Form** Yellow needles**Solubility** Sparingly soluble in water; soluble in ethanol, ether**Melting Point** 145°C**Boiling Point (Calcd.)** $328.9 \pm 27.0^\circ\text{C}$ Pressure: 760 Torr**Synthesis** Synthetic methods^{1–5}**Major Applications** For biosensor design,⁶ drug delivery⁷**Safety/Toxicity** Toxicity,⁸ toxicology,⁹ ecotoxicity,¹⁰ toxic actions,¹¹ mutagenicity¹²**References**

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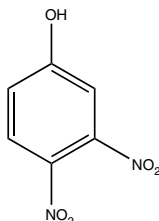
δ -DINITROPHENOL

Other Names 3,4-DNP; 3,4-Dinitrophenol; 6,5-Dinitrophenol; Phenol, δ -dinitro-

CA Index Name Phenol, 3,4-dinitro-

CAS Registry Number 577-71-9

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Nitro

Molecular Formula $C_6H_4N_2O_5$

Molecular Weight 184.11

pH Range 4.3–6.3

Color Change at pH Colorless (4.3) to yellow (6.3)

pKa 5.35, 5.42

Physical Form Light yellow needles

Solubility Sparingly soluble in water; soluble in ethanol, ether

Melting Point 134°C

Boiling Point (Calcd.) $418.7 \pm 35.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods^{1–5}

Major Applications Lubricants,⁶ enzyme assay,⁷ antinerve agent,⁸ substrate for enzymes,⁹ in biotechnological process,¹⁰ for biosensor design¹¹

Safety/Toxicity Toxicity,^{12,13} toxicology,¹⁴ ecotoxicity,¹⁵ mutagenicity¹⁶

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2,4-DINITROPHENYLHYDRAZINE

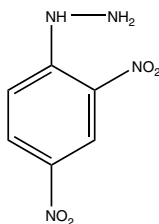
Other Names (2,4-Dinitrophenyl)hydrazine; 1-(2,4-Dinitrophenyl)hydrazine; 1-Hydrazino-2,4-dinitrobenzene; DNPH; NSC 5709

CA Index Name Hydrazine, (2,4-dinitrophenyl)-

CAS Registry Number 119-26-6

Merck Index Number 3283

Chemical Structure



Chemical/Dye Class Miscellaneous

Molecular Formula C₆H₆N₄O₄

Molecular Weight 198.14

pH Range 11.0–12.5

Color Change at pH Yellow (11.0) to brown (12.5)

pKa 12.1

Physical Form Red crystals

Solubility Slightly soluble in water, ethanol

Melting Point 200°C

Boiling Point (Calcd.) 378.6 ± 32.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Fuel cells,³ detecting microorganisms,⁴ antibacterial agent,⁵ treatment of acute and chronic hepatitis,⁶ gynecopathy,⁷ cardiovascular diseases,⁸ cerebrovascular diseases⁸

Safety/Toxicity Bladder toxicity,⁹ carcinogenicity,¹⁰ genotoxicity,¹¹ mutagenicity¹²

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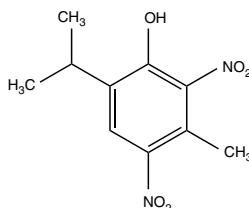
DINITROTHYMOL

Other Names Thymol, 2,6-dinitro-; 2,4-Dinitrothymol; 2,6-Dinitrothymol; 2-Isopropyl-5-methyl-4,6-dinitrophenol; NSC 6767

CA Index Name Phenol, 3-methyl-6-(1-methylethyl)-2,4-dinitro-

CAS Registry Number 303-21-9

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Nitro

Molecular Formula C₁₀H₁₂N₂O₅

Molecular Weight 240.21

pH Range 2.2–3.4

Color Change at pH Colorless (2.2) to yellow (3.4)

pKa 4.86

Physical Form Yellow crystals

Solubility Insoluble in water; soluble in ethanol, methanol

Melting Point >250°C

Boiling Point (Calcd.) 311.7 ± 42.0°C Pressure: 760 Torr

Synthesis Synthetic methods¹

Major Applications Antileishmanial drug¹

Safety/Toxicity Acute oral toxicity²

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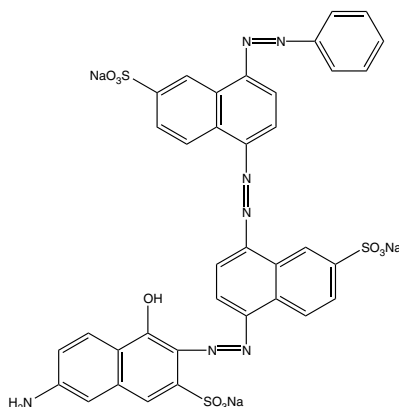
DIRECT BLUE 72

Other Names C.I. Direct Blue 72; C.I. 34145; Diazol Light Blue B; Direct Fast Blue FR

CA Index Name 2-Naphthalenesulfonic acid, 5-[[[(6-amino-1-hydroxy-3-sulfo-2-naphthalenyl)azo]-8-[[4-(phenylazo)-6-sulfo-1-naphthalenyl]azo]-, trisodium salt

CAS Registry Number 6717-34-6

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Azo

Molecular Formula $C_{36}H_{22}N_7O_{10}S_3Na_3$

Molecular Weight 877.76

pH Range 13.0–14.0

Color Change at pH Blue (13.0) to violet (14.0)

pKa 13.8

Physical Form Dark blue powder

Solubility Soluble in water, ethanol

Melting Point $>300^{\circ}\text{C}$

Synthesis Synthetic method¹

Major Applications Coloring paper¹

Safety/Toxicity No data available

Reference

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DIXYLENOLPHTHALEIN

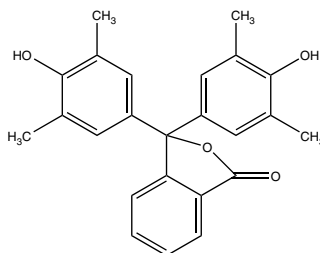
Other Names Phenolphthalein, 3',3'',5',5''-tetramethyl-; 2,6-Dixylenolphthalein

CA Index Name 1(3H)-Isobenzofuranone, 3,3-*bis*(4-hydroxy-3,5-dimethylphenyl)-

CAS Registry Number 3689-45-0

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Phthalein

Molecular Formula C₂₄H₂₂O₄

Molecular Weight 374.43

pH Range 8.5–9.9

Color Change at pH Colorless (8.5) to violet (9.9)

pKa 9.97

Physical Form White powder

Solubility Insoluble in water; soluble in ethanol, methanol

Melting Point 247.5–249.0°C

Boiling Point (Calcd.) 556.6 ± 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–4}

Major Applications Indicator,^{4–6} polymeric alloys,² toothpaste and mouthwash,⁷ disinfectant,⁸ cosmetics,⁹ paints¹⁰

Safety/Toxicity No data available

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E

EOSIN Y

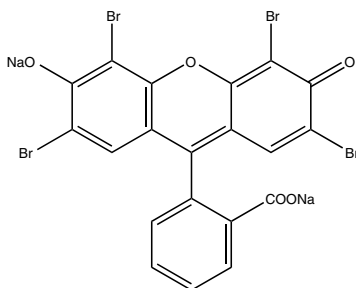
Other Names Eosin Yellowish; Fluorescein, 2',4',5',7'-tetrabromo-, disodium salt; 11445 Red; 11731 Red; 1903 Yellow Pink; Acid Red 87; Aizen Eosine GH; Basacid Red 316; Bromo 4D; Bromo 4DC; Bromo 4DL; Bromo B; Bromo FL; Bromo JPS; Bromo TS; Bromo X 100; Bromo XX; Bromo acid; Bromoeosine; Bromofluoresceic acid; Bromofluorescein; Bronze Bromo; C.I. 45380; C.I. Acid Red 87; Certiquel Eosine; Chugai Ink Red AM 5; D and C Red No. 22; D&C Red 22; D&C Red No. 22; Daiwa Red 103WB; Dawn red; Disodium eosin; Eosin; Eosin A; Eosin OJ; Eosin Y; Eosin YS; Eosin yellow; Eosine; Eosine 3G; Eosine 3Y; Eosine A; Eosine BPC; Eosine BS; Eosine BS-SF; Eosine DA; Eosine DWC 73; Eosine Extra Conc. A. Export; Eosine Extra Yellowish; Eosine FA; Eosine G; Eosine GF; Eosine GH; Eosine J; Eosine K; Eosine K Salt Free; Eosine Lake Red Y; Eosine OJ; Eosine S; Eosine S 13; Eosine Salt Free; Eosine Y; Eosine YB; Eosine YS; Eosine Yellow; Eosine Yellowish; Eosine sodium; Eosine sodium salt; Eosine w/s; Eosine water-soluble; Fenazo Eosine XG; Food Red 103; Hidacid Boiling Bromo; Hidacid Bromo acid regular; Hidacid Dibromo Fluorescein; Hidacid Eosine Soda Salt; Hidacid White Bromo; Irgalite Bronze Red CL; Japan Red 103; Japan Red 230-1; Japan Red 230-2; Japan Red No. 103; Japan Red No. 230-1; Morning red; Orient Water Red 2; Phlox Red Toner X 1354; Phloxine Red 20-7600; Phloxine Toner B; Pure Eosine YY; Red 103; Red No. 103; Red No. 230-1; Sodium eosin; Sodium eosinate; Sodium eosine; Symuler Eosin Toner; Tetrabromofluorescein; Tetrabromofluorescein D; Tetrabromofluorescein S; Tetrabromofluorescein soluble; Toyo Eosine G; Water Red 2

CA Index Name Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 2',4',5',7'-tetrabromo-3',6'-dihydroxy-, disodium salt

CAS Registry Number 17372-87-1

Merck Index Number 3603

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula $C_{20}H_6Br_4O_5Na_2$

Molecular Weight 691.86

pH Range 0.0–3.0

Color Change at pH Yellow or nonfluorescence (0.0) to red or green fluorescence (3.0)

pKa 2.9, 4.5

Physical Form Red crystals

Solubility Freely soluble in water; slightly soluble in ethanol, methanol; insoluble in ether

UV-Visible (λ_{max}) 514 nm

Melting Point 295.5°C

Synthesis Synthetic methods^{1–9}

Major Applications Photovoltaic devices,¹⁰ color filter,¹¹ nanoscale host material,¹² detection of latent fingerprints,¹³ inks,¹⁴ detergents,¹⁵ hair dyes,¹⁶ cosmetics,¹⁷ implantable drug delivery devices,¹⁸ stents,¹⁹ diagnosis of breast lesions,²⁰ labeling nucleic acids,²¹ detecting proteins,²² stress biomarkers,²³ phosphoprotein,²⁴ breast cancer metastases,²⁵ antimicrobial agent,²⁶ treatment of burns,²⁷ endodontic,²⁸ diabetes,²⁹ obesity,²⁹ cancer,³⁰ radiochemotherapy,³¹ DNA sequencing,³² gene expression profiling,³³ wound healing promoters^{34,35}

Safety/Toxicity Acute toxicity,³⁶ mutagenicity,³⁷ phototoxicity³⁸

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ERYTHROSIN B

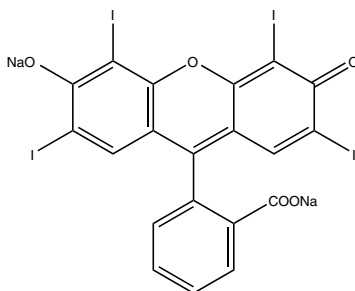
Other Names Fluorescein, 2',4',5',7'-tetraiodo-, disodium salt; 1427 Red; 1671 Red; 2',4',5',7'-Tetraiodofluorescein disodium salt; 2,4,5,7-Tetraiodofluorescein disodium salt; Acid Red 51; Aizen Erythrosine; Aizen Food Red 3; C.I. 45430; C.I. Acid Red 51; C.I. Food Red 14; Calco-cid Erythrosine N; Canacert Erythrosine BS; Ceplac; Cilefa Pink B; D and C Red No. 3; D&C Red No. 3; Dolkwal Erythrosine; E 127; Edicol Supra Erythrosin AS; Edicol Supra Erythrosine A; Erythrosin; Erythrosin B; Erythrosin B sodium salt; Erythrosin BS; Erythrosine; Erythrosine 3B; Erythrosine B-FO; Erythrosine BS; Erythrosine Bluish; Erythrosine Extra; Erythrosine Extra Conc. A Export; Erythrosine Extra Pure A; Erythrosine I; Erythrosine K-FO; Erythrosine TB; Erythrosine TB Extra; Erythrosine extra bluish; FD and C Red 3; FD and C Red No. 3; FD&C Red No. 3; FDC Red 3; FDC Red 3 dye; Food Color Red 3; Food Dye Red 3; Food Red 14; Food Red 3; Food Red No. 3; Hexacert Red No. 3; Hexacol Erythrosine BS; Japan Red 3; Japan Red No. 3; Maple Erythrosine; New Pink Bluish Geigy; Red 1799; S 887; Synerid; Tetraiodofluorescein sodium salt; Usacert Red No. 3

CA Index Name Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-dihydroxy-2',4',5',7'-tetraiodo-, disodium salt

CAS Registry Number 16423-68-0

Merck Index Number 3693

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula C₂₀H₆I₄O₅Na₂

Molecular Weight 879.86

pH Range 2.5–4.0

Color Change at pH Nonfluorescence (2.5) to light green or reddish fluorescence (4.0)

pKa 4.1

Physical Form Brown powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 525 nm

Melting Point >250°C

Synthesis Synthetic methods¹⁻⁸

Major Applications Color filter,⁹ light emitting diodes,¹⁰ nanosensors,¹¹ imaging materials,¹² inks,¹³ paints,¹⁴ colored bubbles,¹⁵ detergents,¹⁶ cleaners,¹⁷ cosmetics,¹⁸ oral care agent,¹⁹ hair dyes,²⁰ anti-septic,²¹ treatment of burns,²² diabetes,²³ obesity,²³ cancer,²⁴ viral diseases,²⁵ radiochemotherapy,²⁶ photodynamic therapy²⁷

Safety/Toxicity Acute toxicity,²⁸ carcinogenicity,²⁹ cytotoxicity,³⁰ embryotoxicity,³¹ genotoxicity,³² mutagenicity,³³ reproductive toxicity,³⁴ neurotoxicity,³⁴ teratogenicity³⁵

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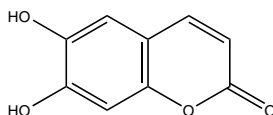
ESCULETIN

Other Names Coumarin, 6,7-dihydroxy-; Esculetin; 6,7-Dihydroxy-2-benzopyrone; 6,7-Dihydroxycoumarin; Aesculetin; Aesculetine; Cichorigenin; Cichoriin aglycon; Esculetol; Esculin aglycon; NSC 26428; Esculetin

CA Index Name 2H-1-Benzopyran-2-one, 6,7-dihydroxy-

CAS Registry Number 305-01-1

Merck Index Number 3697

Chemical Structure

Chemical/Dye Class Fluorescent, Coumarin

Molecular Formula C₉H₆O₄

Molecular Weight 178.14

pH Range 1.5–2.0

Color Change at pH Weak blue fluorescence (1.5) to strong blue fluorescence (2.0)

pKa 1.71

Physical Form Light yellow powder

Solubility Almost insoluble in boiling water, ether; soluble in hot ethanol, glacial acetic acid

Melting Point 272–274°C

Boiling Point (Calcd.) 469.7 ± 45.0 °C Pressure: 760 Torr

Synthesis Synthetic methods^{1–10}

Major Applications Herbicides,¹¹ cosmetics,¹² teeth whitening agent,¹³ antiinflammatory,¹⁴ antifungal,¹⁵ antibacterial,¹⁵ antiviral,¹⁶ treating drug-induced weight gain,¹⁷ neurodegenerative and blood coagulation disorders,¹⁸ cancer,¹⁹ amyloidosis,²⁰ skin impairments and baldness²¹

Safety/Toxicity Cytotoxicity,²² mutagenicity²³

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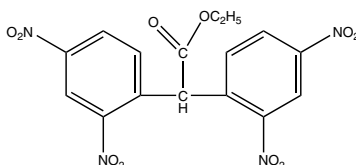
ETHYL *BIS*-(2,4-DINITROPHENYL)ACETATE

Other Names Acetic acid, *bis*(2,4-dinitrophenyl)-, ethyl ester; Ethyl *bis*(2,4-dinitrophenyl)acetate; NSC 8659; *Bis*(2,4-dinitrophenyl)-acetic acid ethyl ester

CA Index Name Benzeneacetic acid, α -(2,4-dinitrophenyl)-2,4-dinitro-, ethyl ester

CAS Registry Number 5833-18-1

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Miscellaneous, Nitro

Molecular Formula C₁₆H₁₂N₄O₁₀

Molecular Weight 420.29

pH Range 7.5–9.1

Color Change at pH Colorless (7.5) to deep blue (9.1)

pKa 8.3

Physical Form Pale yellow crystals

Solubility Insoluble in water; soluble in ethanol, acetone

Melting Point 150–153°C

Boiling Point (Calcd.) 629.3 ± 55.0 °C Pressure: 760 Torr

Synthesis Synthetic method^{1,2}

Major Applications Imaging materials,³ microcapsule toner,⁴ electrophotographic toner,⁵ decoder system,⁶ inks,⁷ paints,⁸ adhesives,⁹ identification of organic solvents¹⁰

Safety/Toxicity No data available

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ETHYL GREEN

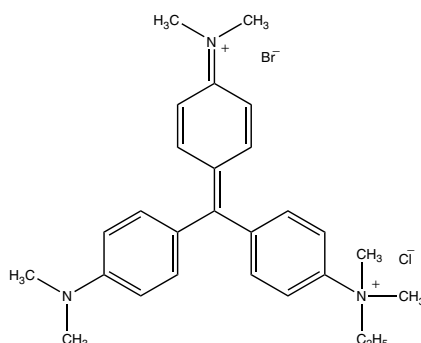
Other Names Ammonium, [α -[*p*-(dimethylamino)phenyl]- α -[4-(dimethyliminio)-2,5-cyclohexadien-1-ylidene]-*p*-tolyl]-ethyl dimethyl-, bromide, chloride; [α -[*p*-(Dimethylamino)-phenyl]- α -[4-(methyliminio)-2,5-cyclohexadien-1-ylidene]-*p*-tolyl]ethyl dimethyl ammonium bromide, methochloride; Ethyl green

CA Index Name Benzenaminium, 4-[[4-(dimethylamino)phenyl][4-(dimethyliminio)-2,5-cyclohexadien-1-ylidene]methyl]-*N*-ethyl-*N,N*-dimethyl-, bromide chloride

CAS Registry Number 14855-76-6

Merck Index Number 6082

Chemical Structure



Note: The traditional Methyl Green has not manufactured for decades. The dye sold as Methyl Green is more accurately described as Ethyl Green. Both, Methyl Green and Ethyl Green are sold as double zinc salts.

Chemical/Dye Class Triphenylmethane

Molecular Formula $C_{27}H_{35}N_3BrCl$

Molecular Weight 516.94

pH Range 0.1–2.3

Color Change at pH Yellow (0.1) to Greenish-blue (2.3)

Physical Form Green power

Solubility Soluble in water, ethanol; insoluble in xylene

UV-Visible (λ_{max}) 635 nm, 420 nm

Melting Point >300°C

Synthesis Synthetic method¹

Major Applications Inks,² nucleic acid stain,³ antifungal agent⁴

Safety/Toxicity Mutagenicity⁵

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ETHYL ORANGE

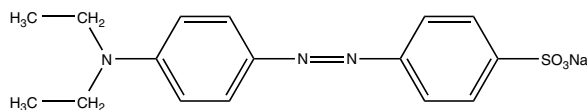
Other Names Benzenesulfonic acid, *p*-[[*p*-(diethylamino)phenyl]azo]-, sodium salt; Ethyl orange sodium salt; Sodium 4-[[4-(diethylamino)phenyl]azo]benzenesulfonate

CA Index Name Benzenesulfonic acid, 4-[[4-(diethylamino)phenyl]azo]-, sodium salt

CAS Registry Number 62758-12-7

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula C₁₆H₁₈N₃O₃SNa

Molecular Weight 355.39

pH Range 3.4–4.8

Color Change at pH Red (3.4) to yellow (4.8)

pKa 4.34

Physical Form Orange powder

Solubility Very soluble in water; very slightly soluble in ethanol

UV-Visible (λ_{max}) 474 nm

Melting Point >300°C

Synthesis Synthetic method¹

Major Applications Lithographic plate preparation,² holographic storage,³ hybrid materials,⁴ inks,⁵ surface probes,⁶ diagnostic agents for diseases related with amyloid accumulation⁷

Safety/Toxicity No data available

References

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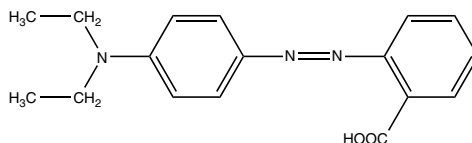
ETHYL RED

Other Names 2-[4-(Diethylamino)phenylazo]benzoic acid; Ethyl Red; NSC 260474

CA Index Name Benzoic acid, 2-[[4-(diethylamino)phenyl]azo]-

CAS Registry Number 76058-33-8

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Azo

Molecular Formula C₁₇H₁₉N₃O₂

Molecular Weight 297.35

pH Range 4.5–6.5

Color Change at pH Red (4.5) to yellow (6.5)

pKa 5.42

Physical Form Red powder

Solubility Almost insoluble in water; slightly soluble in ethanol, soluble in benzene

UV-Visible (λ_{max}) 447 nm

Melting Point 135°C (decompose)

Boiling Point (Calcd.) 496.9 ± 30.0 °C Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Optical materials,^{3–6} photoresists,^{7,8} flexible electronic circuitry,⁹ adhesives,¹⁰ textiles,^{11,12} method for counting leukocytes,¹³ enzyme binding assays,¹⁴ DNA chips¹⁵

Safety/Toxicity No data available

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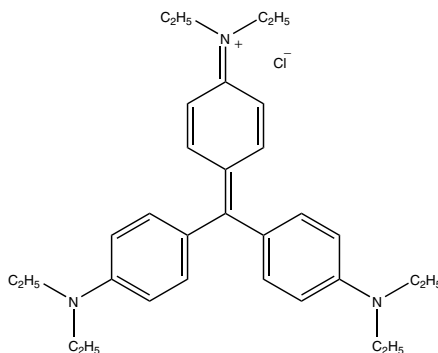
ETHYL VIOLET

Other Names C.I. Basic Violet 4; Ethyl violet; Basic Violet 4; C.I. 42600; Ethyl Violet AX; Ethyl Violet GGA; Ethyl crystal violet; Lowacryl Violet 4; Shikiso Acid Brilliant Blue 6B; *Tris*(*p*-(diethylamino)-phenyl)methylm chloride

CA Index Name Ethanaminium, *N*-[4-[*bis*[4-(diethylamino)phenyl]methylene]-2,5-cyclohexadien-1-ylidene]-*N*-ethyl-, chloride

CAS Registry Number 2390-59-2

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Triphenylmethane

Molecular Formula C₃₁H₄₂N₃Cl

Molecular Weight 492.15

pH Range 0.0–3.5

Color Change at pH Yellow (0.0) to blue (3.5)

Physical Form Olive green powder

Solubility Slightly soluble in water; soluble in ethanol, methanol

UV-Visible (λ_{max}) 596 nm

Melting Point >250°C

Synthesis Synthetic methods^{1,2}

Major Applications Integrated circuits,³ fiber-optic pH sensors,⁴ display device,⁵ inks,⁶ highlighter,⁷ lithographic printing plates,⁸ decoder system,⁹ detergents,¹⁰ hair dyes,¹¹ cosmetics,¹² wound dressing materials,¹³ diagnosis of diseases caused by elemental imbalances,¹⁴ antimicrobial,¹⁵ photochemotherapeutic agent¹⁶

Safety/Toxicity Acute oral toxicity,¹⁷ phototoxicity¹⁸

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F

FLUORESC EIN

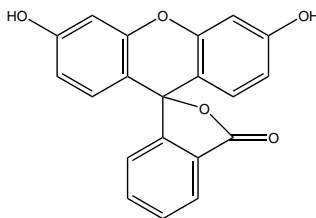
Other Names Fluorescein; 3',6'-Dihydroxyfluoran; 3',6'-Fluorandiol; 3,6-Dihydroxyspiro [xanthene-9,3'-phthalide]; 9-(*o*-Carboxyphenyl)-6-hydroxy-3-isoxanthenone; Benzoic acid, 2-(6-hydroxy-3-oxo-3H-xanthen-9-yl)-; C.I. 45350:1; C.I. Solvent Yellow 94; D and C Yellow No. 7; D&C Yellow No. 7; Fluorescein acid; Japan Yellow 201; Japan Yellow No. 201; NSC 667256; Resorcinolphthalein; Solvent Yellow 94; Yellow fluorescein

CA Index Name Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-dihydroxy-

CAS Registry Number 2321-07-5

Merck Index Number 4159

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula C₂₀H₁₂O₅

Molecular Weight 332.31

pH Range 4.0–6.0

Color Change at pH Pink fluorescence (4.0) to green fluorescence (6.0)

pKa 2.2, 4.4, 6.7

Physical Form Yellowish-red powder

Solubility Insoluble in water, ether, benzene, chloroform; soluble in ethanol, methanol, acetone, ethyl acetate, *N,N*-dimethylformamide

UV-Visible (λ_{max}) 493.5 nm, 496 nm, 460 nm, 515 nm

Melting Point 315°C (decompose)

Boiling Point (Calcd.) 620.8 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–6}

Major Applications Organic light-emitting diode,⁷ nanoparticles,⁸ liquid crystal display,⁹ oil products,¹⁰ lip make-up,¹¹ nucleic acid synthesis, amplification, sequencing and cloning,¹² diagnosis of diabetic retinopathy,¹³ detecting yeast,¹⁴ multidrug resistance,¹⁵ proteins,¹⁶ antiHCV antibodies,¹⁷ target genes,¹⁸ enzymatic activity,¹⁹ nerve agent,²⁰ nucleic acid sequences,²¹ imaging lung cancer,²² prostate cancer²³

Safety/Toxicity Adverse reaction,²⁴ acute toxicity,²⁵ cellular toxicity,²⁶ cytotoxicity,²⁷ mutagenicity,²⁸ phototoxicity²⁹

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FLUORESC EIN DIACETATE (FDA)

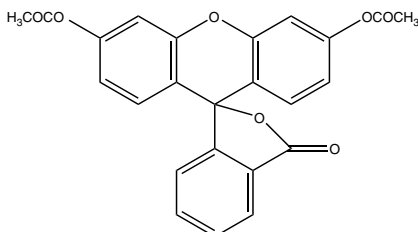
Other Names Fluorescein, diacetate; 3',6'-Diacetylfluorescein; Fluorescein 3',6'-diacetate; MFCD 5062; NSC 4726; NSC 667259

CA Index Name Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-bis(acetyloxy)-

CAS Registry Number 596-09-8

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula C₂₄H₁₆O₇

Molecular Weight 416.38

pH Range 6.0–7.2

Color Change at pH Weak green fluorescence (6.0) to strong green fluorescence (7.2)

pKa 6.4

Physical Form Light yellow powder

Solubility Slightly soluble in water, ethanol; soluble in methanol, *N,N*-dimethylformamide

UV-Visible (λ_{max}) 490 nm

Melting Point 200–203°C

Boiling Point (Calcd.) 604.7 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–3}

Major Applications LED devices,⁴ petroleum markers,¹ identifying cancerous cells,⁵ detecting bacteria,⁶ virus,⁷ mitochondrial function in neurons,⁸ target molecules,⁹ living cells,¹⁰ viable *Giardia* cysts in water samples,¹¹ apoptosis,¹² evaluating live/dead state of algae,¹³ measurement of total microbial activity in soil,¹⁴ treating ischemia¹⁵

Safety/Toxicity Cytotoxicity,¹⁶ ecotoxicity,¹⁷ neurotoxicity,¹⁸ phytotoxicity¹⁹

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FLUORESCEIN DISODIUM SALT

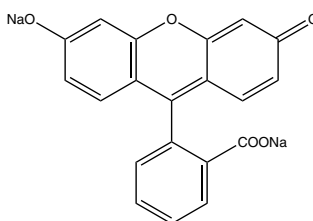
Other Names Fluorescein, disodium salt; Fluorin; 11824 Yellow; 12417 Yellow; 3058 Uranine; Acid Yellow 73; Aizen Uranine; Basacid Yellow 226; C.I. 45350; C.I. Acid Yellow 73; Calcocid Uranine B 4315; Certiqua Fluoresceine; D & C Yellow 8; D and C Yellow No. 8; D&C Yellow No. 8; Disodium fluorescein; Fluo-rectal; Fluor-I-Strip; Fluorescein LT; Fluorescein Sodium B.P; Fluorescein disodium; Fluorescein sodium; Fluorescein sodium salt; Fluorescite; Flurenate; Ful-Glo; Furanium; Hidacid Uranine; Japan Yellow 202(1); Obiturine; Resorcinol phthalein sodium; Sodium fluorescein; Sodium fluoresceinate; Soluble Fluorescein; Soluble Fluoresceine BPS; Uranin; Uranin A; Uranin Conc; Uranin S; Uranine; Uranine A; Uranine A extra; Uranine O; Uranine SS; Uranine WSS

CA Index Name Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-dihydroxy-, disodium salt

CAS Registry Number 518-47-8

Merck Index Number 4159

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula $C_{20}H_{10}O_5Na_2$

Molecular Weight 376.28

pH Range 4.0–6.0

Color Change at pH Pink fluorescence (4.0) to green fluorescence (6.0)

pKa 2.2, 4.4, 6.7

Physical Form Orange-red powder

Solubility Freely soluble in water; slightly soluble in ethanol

UV-Visible (λ_{max}) 491 nm, 493.5 nm, 490 nm

Melting Point >300°C

Synthesis Synthetic methods^{1–4}

Major Applications Nanolithography,⁵ nanoparticles,⁶ thin films,⁷ fuel cells,⁸ inks,⁹ laser,¹⁰ colored bubbles,¹¹ cleansing products,¹² identifying leaks in coolant,¹³ suntanning agent,¹⁴ hair dyes,¹⁵ cosmetics,¹⁶ dermatology,¹⁷ dental material,¹⁸ diagnosis of diabetic retinopathy,¹⁹ antitumor agent²⁰

Safety/Toxicity Acute and chronic toxicity,²¹ ecotoxicity,²² hemorheological effects,²³ toxicity to insects,²⁴ mutagenicity,²⁵ carcinogenicity,²⁵ chromosome aberration,²⁶ phototoxicity²⁷

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FLUORESC EIN-5-ISOTHIOCYANATE (FITC)

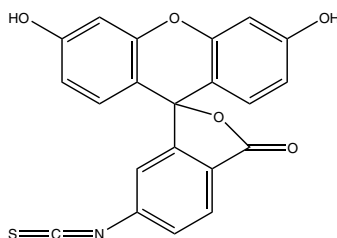
Other Names Fluorescein, 5-isothiocyanato-; 5-Isothiocyanatofluorescein; FITC isomer I; Fluorescein 5-isothiocyanate; Fluorescein isothiocyanate isomer 1; Fluorescein isothiocyanate isomer I; Fluorescein-5-isothiocyanate

CA Index Name Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-dihydroxy-5-isothiocyanato-

CAS Registry Number 3326-32-7

Merck Index Number 4089

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula C₂₁H₁₁NO₅S

Molecular Weight 389.38

pH Range 6.0–7.2

Color Change at pH Weak green fluorescence (6.0) to strong green fluorescence (7.2)

pKa 2.2, 4.4, 6.7

Physical Form Orange powder

Solubility Insoluble in water; soluble in ethanol, acetone, *N,N*-dimethylformamide

UV-Visible (λ_{max}) 490 nm

Melting Point >360°C

Boiling Point (Calcd.) 708.6 ± 60.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–5}

Major Applications Magnetic nanowires,⁶ immunoassays,⁷ analyzing proteins,⁸ identifying chromosomes,⁹ diagnosis of cancer,¹⁰ kidney diseases,¹¹ detecting pathogens,¹² genes,¹³ *Salmonella* cells,¹⁴ toxoplasmosis,¹⁵ enzyme-mediated nucleic acid cleavage,¹⁶ surface molecules on colorectal cancers,¹⁷ treating cancer,¹⁸ chronic lymphocytic leukemia¹⁹

Safety/Toxicity Cytotoxicity,²⁰ genotoxicity,²¹ phototoxicity²²

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FLUOREXON

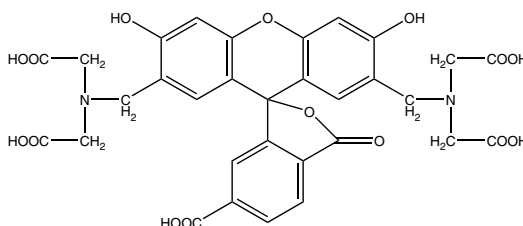
Other Names Fluorescein, 2',7'-bis[[bis(carboxymethyl)amino]methyl]-; Spiro[isobenzofuran-1(3H),9'-[9H]xanthene], glycine deriv.; 2,7-Bis[*N,N*-bis(carboxymethyl)aminomethylene]-fluorescein; Acetic acid, [(3',6'-dihydroxy-2',7'-fluorandiyl)bis-(methylenenitrilo)]tetra-; Calcein; Fluorescein complexon; Fluorexon; NSC 298193; Oftasceine

CA Index Name Glycine, *N,N'*-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-2',7'-diyl)bis(methylene)]bis[*N*-(carboxymethyl)-

CAS Registry Number 1461-15-0

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula C₃₀H₂₆N₂O₁₃

Molecular Weight 622.53

pH Range 6.0–7.2

Color Change at pH Weak green fluorescence (6.0) to strong green fluorescence (7.2)

pKa 6.67

Physical Form Orange powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 494 nm

Melting Point >250°C

Boiling Point (Calcd.) 952.7 ± 65.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–6}

Major Applications Chemical–mechanical polishing,^{7,8} stabilizing liposomes,⁹ cell motility assay,¹⁰ detecting nucleic acids,¹¹ virus,¹² screening safety of gastric mucosa,¹³ MDR inhibitors,¹⁴ drug delivery,¹⁵ imaging atherosclerotic plaque¹⁶

Safety/Toxicity Cytotoxicity,¹⁷ exitotoxicity¹⁸

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G

GALLEIN

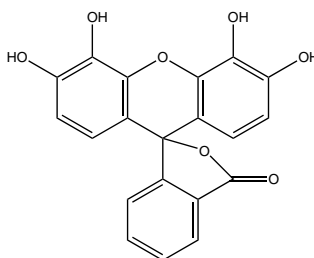
Other Names Gallein; Alizarine violet; C.I. 45445; C.I. Mordant Violet 25; Mordant Violet 25; NSC 56445; NSC 622478; NSC 8668; Pyrogallolphthalein

CA Index Name Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',4',5',6'-tetrahydroxy-

CAS Registry Number 2103-64-2

Merck Index Number 4344

Chemical Structure



Chemical/Dye Class Miscellaneous, Xanthene

Molecular Formula C₂₀H₁₂O₇

Molecular Weight 364.31

pH Range 3.8–6.6;
10.6–13.0

Color Change at pH Yellow (3.8) to rose-red (6.6)
Pink (10.6) to violet (13.0)

pKa 5.99

Physical Form Brownish-red powder

Solubility Almost insoluble in water, benzene, chloroform; soluble in ethanol, acetone

UV-Visible (λ_{max}) 526 nm

Melting Point >300°C

Boiling Point (Calcd.) 687.4 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–7}

Major Applications Organic light emitting devices (OLED),⁸ semiconductors,^{9,10} photoresists,^{11,12} lithographic printing plates,¹³ method for ozone determination,¹⁴ treatment of wastewater,¹⁵ determination of silver,¹⁶ nail polish,¹⁷ monitoring sterilization,¹⁸ determination of proteins,¹⁹ induce apoptosis in cancer cells,²⁰ treatment of cancer cells,²¹ antiHIV agent,²² diagnosis and treatment of amyloidosis,²³ cancer chemo preventive activity,²⁴ drug design,²⁵ inhibition of influenza virus²⁶

Safety/Toxicity No data available

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GENTIAN VIOLET

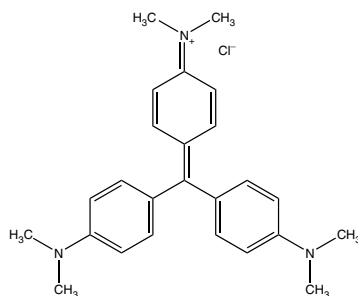
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CA Index Name Methanaminium, N-[4-*bis*[4-(dimethylamino)phenyl]methylene]-2,5-cyclohexadien-1-ylidene]-N-methyl-, chloride

CAS Registry Number 548-62-9

Merck Index Number 4395

Chemical Structure



Chemical/Dye Class Triphenylmethane

Molecular Formula C₂₅H₃₀N₃Cl

Molecular Weight 407.99

pH Range 0.0–2.0

Color Change at pH Yellow (0.0) to blue-violet (2.0)

pKa 9.4

Physical Form Green to yellowish-green powder

Solubility Soluble in water, acetone, chloroform; very soluble in ethanol; practically insoluble in ether; insoluble in xylene

UV-Visible (λ_{max}) 590 nm

Melting Point 205–215°C (decompose)

Synthesis Synthetic methods^{1–12}

Major Applications Photoresists,¹³ lithographic printing plate,¹⁴ printed circuit board,¹⁵ inks,¹⁶ detergent,¹⁷ hair dyes,¹⁸ shampoo,¹⁹ drug screening method,²⁰ bone cement preparation method,²¹ treating microorganisms,²² hemorrhoids,²³ antifungal,²⁴ antibacterial,²⁵ antimalarial agent,²⁶ dental application²⁷

Safety/Toxicity Acute oral toxicity,²⁸ chronic toxicity,^{29,30} carcinogenicity,^{29,30} cytotoxicity,³¹ genotoxicity,³² mutagenicity,^{33,34} ototoxicity,³⁵ percutaneous toxicity,³⁶ phototoxicity³⁷

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GENTIAN VIOLET B

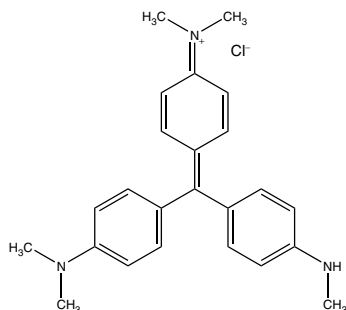
Other Names Methyl violet; Aizen Methyl Violet BB; Aizen Methyl Violet Pure Special; Basic Violet 1; Basic Violet 5BN; Basic Violet K; Basonyl Violet 600; C Ext. Violet 5; C.I. 42535; Gentian Violet B; Methyl Violet 2B; Methyl Violet 6B; Methyl Violet B; Methyl Violet BB; Methyl Violet FN; Methyl Violet N; Methyl Violet Pure Special; Methyl Violet pure SP; Paris Violet R; Pyoktanin blue; Pyoktaninum coeruleum; Violet Powder H 2503

CA Index Name C.I. Basic Violet 1

CAS Registry Number 8004-87-3

Merck Index Number Not listed

Chemical Structure It is a mixture of *N*-pentamethyl (as shown) and *N*-hexamethyl (which is Crystal Violet) *p*-rosaniline chlorides



Chemical/Dye Class Triphenylmethane

Molecular Formula Mixture of tetra-, penta-, and hexamethyl *p*-rosaniline chlorides

Molecular Weight Mixture of tetra-, penta-, and hexamethyl *p*-rosaniline chlorides

pH Range 0.15–3.2

Color Change at pH Yellow (0.15) to violet (3.2)

Physical Form Green crystals

Solubility Soluble in water, ethanol, chloroform; insoluble in ether, xylene

UV-Visible (λ_{max}) 584 nm

Melting Point 137°C (decompose)

Synthesis Synthetic methods^{1–6}

Major Applications Display device,^{7,8} photoresists,⁹ solar cells,¹⁰ inks,^{11,12} highlighters,¹³ rubber,¹⁴ lithium battery,¹⁵ petroleum products,¹⁶ leak detection method,¹⁷ decoder system,¹⁸ packaging materials,¹⁹ hair dyes,²⁰ cosmetics,²¹ wound dressing materials,²² antitumor agent,²³ determination of nucleic acids²⁴

Safety/Toxicity Acute toxicity,²⁵ carcinogenicity,²⁶ toxicity to aquatic microbes,²⁷ mutagenicity²⁸

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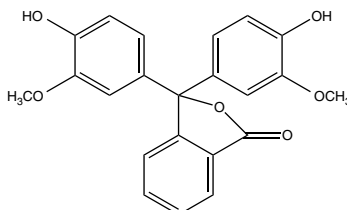
GUAIACOLPHTHALEIN

Other Names Phenolphthalein, 3',3''-dimethoxy-; 3',3''-Dimethoxyphenolphthalein; Guaiacolphthalein

CA Index Name 1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxy-3-methoxyphenyl)-

CAS Registry Number 467-25-4

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Phthalein

Molecular Formula C₂₂H₁₈O₆

Molecular Weight 378.37

pH Range 8.4–10.2

Color Change at pH Colorless (8.4) to violet-blue (10.2)

pKa 9.7

Physical Form White powder

Solubility Insoluble in water; soluble in ethanol, methanol

Melting Point >300°C

Boiling Point (Calcd.) 602.2 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic method^{1,2}

Major Applications Toner,³ toothpaste & mouthwash,⁴ disinfectant,⁵ cosmetics,⁶ paints⁷

Safety/Toxicity No data available

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H

HARMINE

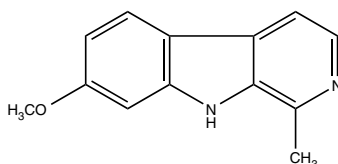
Other Names 1-Methyl-7-methoxy- β -carboline; 7-Methoxy-1-methyl-9H-pyrido[3,4-b]indole; Banisterin; Banisterine; Harmin; Harmine; Leucoharmine; Telepathin; Telepathine; Yagein; Yageine

CA Index Name 9H-Pyrido[3,4-b]indole, 7-methoxy-1-methyl-

CAS Registry Number 442-51-3

Merck Index Number 4616

Chemical Structure



Chemical/Dye Class Fluorescent, Heterocyclic

Molecular Formula C₁₃H₁₂N₂O

Molecular Weight 212.25

pH Range 7.2–8.9

Color Change at pH Blue fluorescence (7.2) to yellow fluorescence (8.9)

pKa 7.7

Physical Form White to off-white crystals

Solubility Slightly soluble in water, ethanol, ether, chloroform

UV-Visible (λ_{max}) 241 nm, 301 nm, 336 nm

Melting Point 261°C (decompose)

Boiling Point (Calcd.) 421.4 $\pm$ 40.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–11}

Major Applications Inks,¹² antitumor agents,^{1,3,7,8,13–15} inhibition of cell proliferation,¹⁶ blocking breast and prostate cancer cells,¹⁷ tracer for ductal pancreatic cancer,¹⁸ DNA binding properties,¹⁹ treatment of neoplasia,²⁰ antioxidants,²¹ therapy of depression,²² antileishmanial agent,^{23,24} treatment of parkinsonism,^{25,26} antiAIDS agents,^{3,27} antihypoxia agents,²⁸ drugs,²⁹ treatment of dependency disorder,³⁰ psychiatric and neurological illness,³¹ antibiotics,³² antimalarial agents.³³

Safety/Toxicity Neurotoxicity,^{7,34,35} nephrotoxicity,³⁵ cytotoxicity,³⁶ genotoxicity,^{37–39} hepatocarcinogenicity,⁴⁰ mutagenicity,⁴¹ hepatotoxicity.⁴²

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HEMATOXYLIN

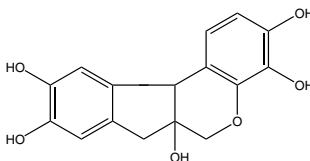
Other Names Benz[b]indeno[1,2-d]pyran-3,4,6a,9,10(6H)-pentol, 7,11b-dihydro; Benz[b]indeno[1,2-d]pyran-3,4,6a,9,10(6H)-pentol, 7,11b-dihydro, (6aS-cis)-; (+)-Hematoxylin; Haematoxylin; Hematoxylin; Hematoxyline; Hydroxybrazilin; Hydroxybrazilin; NSC 270085

CA Index Name Benz[b]indeno[1,2-d]pyran-3,4,6a,9,10(6H)-pentol, 7,11b-dihydro, (6aS,11bR)-

CAS Registry Number 517-28-2

Merck Index Number 4637

Chemical Structure



Chemical/Dye Class Miscellaneous, Polymethine, Flavone

Molecular Formula C₁₆H₁₄O₆

Molecular Weight 302.28

pH Range 0.0–1.0;

5.0–6.0

Color Change at pH Red (0.0) to yellow (1.0)

Pale yellow (5.0) to violet (6.0)

pKa 6.7

Physical Form Tan powder

Solubility Soluble in water, ethanol, ethylene glycol, methyl cellosolve

UV-Visible (λ_{max}) 292 nm, 445 nm, 560 nm

Melting Point 200°C (decompose)

Boiling Point (Calcd.) 579.9 ± 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–6}

Major Applications Plasma displays,⁷ textiles,⁸ hair dyes,⁹ identifying fresh and stale rice,¹⁰ diagnosing cancer progression,¹¹ cervical disease,¹² central nervous system malfunctions,¹³ detecting genes,¹⁴ breast cancer,¹⁵ collagen in a tissue sample,¹⁶ apoptosis,¹⁷ demyelinating diseases,¹⁸ antigens,¹⁹ treatment of age-related macular degeneration,²⁰ burns,²¹ prostate cancer,²² diabetes and obesity,²³ viral diseases,²⁴ neoplasms,²⁵ peripheral neural and vascular ailments,²⁶ skin disorders,²⁷ biotechnological applications,²⁸ reference standard materials for cytology, histology and immunohistochemistry²⁹

Safety/Toxicity Carcinogenicity,³⁰ genotoxicity,³¹ mutagenicity,³² neurotoxicity³³

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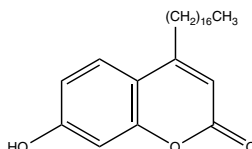
4-HEPTADECYL-7-HYDROXYCOUMARIN

Other Names Coumarin, 4-heptadecyl-7-hydroxy-; 4-Heptadecyl-7-hydroxycoumarin; 4-Heptadecylumbelliferone

CA Index Name 2H-1-Benzopyran-2-one, 4-heptadecyl-7-hydroxy-

CAS Registry Number 26038-83-5

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Fluorescent, Coumarin

Molecular Formula C₂₆H₄₀O₃

Molecular Weight 400.59

pH Range 7.9–9.9

Color Change at pH Weak blue fluorescence (7.9) to strong blue fluorescence (9.9)

pKa 8.9

Physical Form Off-white solid

Solubility Insoluble in water; soluble in ethanol, N,N-dimethylformamide, dimethyl sulfoxide

UV-Visible (λ_{max}) 325 nm, 366 nm

Melting Point 95°C

Boiling Point (Calcd.) 544.7 ± 45.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Fluorescent probes,^{3,4} monolayer assemblies,⁵ lipoplex electrostatics,⁶ opto-acoustic contrast agents⁷

Safety/Toxicity No data available

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HEPTAMETHOXY RED

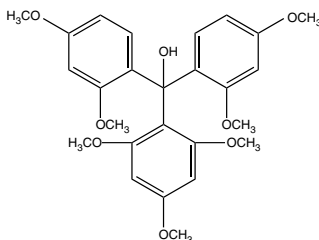
Other Names Carbinol, *bis*(2,4-dimethoxyphenyl)(2,4,6-trimethoxyphenyl)-; Heptamethoxy red

CA Index Name Benzenemethanol, α,α -*bis*(2,4-dimethoxyphenyl)-2,4,6-trimethoxy-

CAS Registry Number 80202-76-2

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Triphenylmethane

Molecular Formula C₂₆H₃₀O₈

Molecular Weight 470.51

pH Range 5.0–7.0

Color Change at pH Red (5.0) to colorless (7.0)

pKa 5.9

Physical Form White crystalline powder

Solubility Insoluble in water; soluble in ethanol

Melting Point 149°C

Boiling Point (Calcd.) 652.2 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Recording materials,³ inks^{4,5}

Safety/Toxicity No data available

References

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HEXAMETHOXY RED

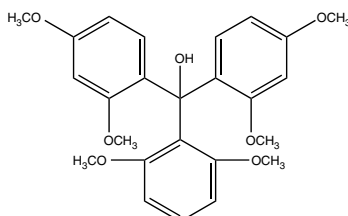
Other Names Hexamethoxytriphenylcarbinol

CA Index Name Benzenemethanol, α,α -bis(2,4-dimethoxyphenyl)-2,6-dimethoxy-

CAS Registry Number 50814-92-1

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Triphenylmethane

Molecular Formula C₂₅H₂₈O₇

Molecular Weight 440.44

pH Range 2.6–4.6

Color Change at pH Reddish-pink (2.6) to colorless (4.6)

pKa 3.3

Physical Form White crystalline powder

Solubility Insoluble in water, soluble in ethanol

Melting Point 147°C

Synthesis Synthetic method¹

Major Applications Inks^{2–4}

Safety/Toxicity No data available

References

1. Lund, H. Methoxy-substituted triphenyl carbinols and their salts. *J. Am. Chem. Soc.* **1927**, *49*, 1346–1360.
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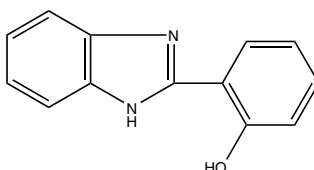
o-HYDROXYPHENYLBENZIMIDAZOLE

Other Names Phenol, o-2-benzimidazolyl-; 2-(1H-Benzimidazol-2-yl)phenol; 2-(2'-Hydroxyphenyl)benzimidazole; 2-(2-Benzimidazolyl)phenol; 2-(2-Hydroxyphenyl)-1H-benzimidazole; 2-(2-Hydroxyphenyl)-benzimidazole; 2-(o-Hydroxyphenyl)-benzimidazole; HBI; NSC 32819

CA Index Name Phenol, 2-(1H-benzimidazol-2-yl)-

CAS Registry Number 2963-66-8

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Fluorescent

Molecular Formula C₁₃H₁₀N₂O

Molecular Weight 210.23

pH Range -9.9-

Color Change at pH Nonfluorescence (<9.9) to blue-violet fluorescence (9.9)

pKa 9.23

Physical Form White to tan crystals

Solubility Insoluble in water; soluble in ethanol

UV-Visible (λ_{max}) 245 nm, 300 nm

Melting Point 240–242°C

Boiling Point (Calcd.) 444.2 ± 47.0°C Pressure: 760

Synthesis Synthetic methods¹⁻⁶

Major Applications Optical devices,⁷ photography,⁸ plastic scintillation applications,⁹ fungicide,¹⁰ antiviral agent,¹¹ antiinflammatory agent,¹² antibacterial agent¹²

Safety/Toxicity Acute toxicity¹³

References

1. Ma, H.; Wang, Y.; Wang, J. A simple KHSO₄-promoted synthesis of 2-aryl-substituted benzimidazoles by oxidative condensation of aldehydes with o-phenylenediamine. *Heterocycles* **2006**, *68*, 1669–1673.
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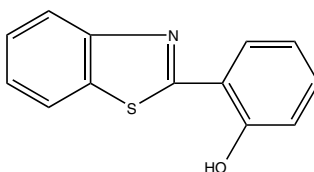
o-HYDROXYPHENYLBENZOTHAZOLE

OtherNames Phenol, o-2-benzothiazolyl-; 2-(2'-Hydroxyphenyl)benzothiazole; 2-(2-Benzothiazolyl)phenol; 2-(2-Hydroxyphenyl)benzothiazole; 2-(o-Hydroxyphenyl)benzothiazole; HBT; NSC 5051; NSC 58548

CA Index Name Phenol, 2-(2-benzothiazolyl)-

CAS Registry Number 3411-95-8

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Fluorescent

Molecular Formula C₁₃H₉NOS

Molecular Weight 227.28

pH Range -9.3-

Color Change at pH Nonfluorescence (<9.3) to blue-green fluorescence (9.3)

pKa 8.21

Physical Form Solid

Solubility Insoluble in water; soluble in ethanol

Melting Point 130–132°C

Boiling Point (Calcd.) 402.2 ± 47.0°C Pressure: 760

Synthesis Synthetic methods^{1–6}

Major Applications Organic light emitting devices,^{7,8} electroluminescent devices,^{9,10} laser dyes,¹¹ photography,¹² plastic scintillation applications,¹³ herbicides,¹⁴ eyeglass lenses,¹⁵ cosmetics¹⁶

Safety/Toxicity Endocrine disrupters¹⁷

References

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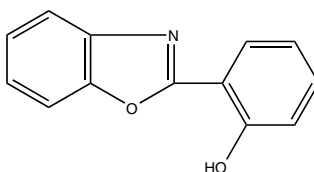
o-HYDROXYPHENYLBENZOXAZOLE

Other Names Phenol, *o*-2-benzoxazolyl-; 2-(1,3-Benzoxazol-2-yl)phenol; 2-(2'-Hydroxyphenyl)benzoxazole; 2-(2-Hydroxyphenyl)benzoxazole; 2-(*o*-Hydroxyphenyl)benzoxazole; HBO; NSC 403545; NSC 5423; *o*-2-Benzoxazolylphenol

CA Index Name Phenol, 2-(2-benzoxazolyl)-

CAS Registry Number 835-64-3

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Fluorescent

Molecular Formula C₁₃H₉NO₂

Molecular Weight 211.22

pH Range -9.3-

Color Change at pH Nonfluorescence (<9.3) to blue-violet fluorescence (9.3)

pKa 8.04

Physical Form Solid

Solubility Insoluble in water; soluble in ethanol

Melting Point 125–126°C

Boiling Point 338°C

Synthesis Synthetic methods¹⁻⁸

Major Applications Electroluminescent devices,^{9,10} reflective films,¹¹ sensors,¹² plastic scintillation applications,¹³ antitumor agent,¹⁴ antibacterial agent¹⁴

Safety/Toxicity No data available

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INDIGO CARMINE

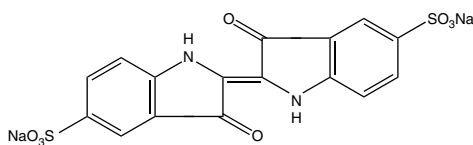
Other Names C.I. Acid Blue 74; [$\Delta 2,2'$ -Biindoline]-5,5'-disulfonic acid, 3,3'-dioxo-, disodium salt; 12070 Blue; 1311 Blue; 5,5'-Indigodisulfonic acid disodium salt; A.F. Blue No. 2; Acid Blue 74; Acid Blue W; Acid Leather Blue IC; Airedale Blue IN; Amacid Brilliant Blue; Aniline Carmine Powder; Ariavit Indigo Carmine; Atul Indigo Carmine; Bucacid Indigotine B; C.I. 73015; C.I. 75781; C.I. Food Blue 1; C.I. Natural Blue 2; Canacert Indigo Carmine; Carmine Blue; Cilefa Blue R; Disodium 5,5'-indigodisulfonate; Disodium 5,5'-indigotin disulfonate; Dolkwal Indigo Carmine; E 132; Edicol Supra Blue X; FD & C Blue 2; FD and C Blue 2; FD and C Blue No. 2; FD&C Blue No. 2; Food Blue 1; Food Blue 2; Food Blue No. 1; Food Blue No. 2; Grape Blue A; HD Indigo Carmine; HD Indigo Carmine Supra; Hexacert Blue No. 2; Hexacol Indigo Carmine Supra; Indigo Carmine A; Indigo Carmine AC; Indigo Carmine BP; Indigo Carmine Conc. FQ; Indigo Carmine Powder; Indigo Carmine X; Indigo Extract; Indigo carmine; Indigo carmine NB; Indigotin; Indigotin (solubilized); Indigotine; Indigotine B; Indigotine Blue LZ; Indigotine Carmine; Indigotine Extra Pure A; Indigotine I; Indigotine IA; Indigotine Lake; Indigotine N; Indigotine disodium salt; Indocarmine F; Intense Blue; Japan Blue 2; L Blue Z 5010; Maple Indigo Carmine; Mitsui Indigo Carmine; San-ei Indigo Carmine; Sodium 5,5'-indigodisulfonate; Sodium 5,5'-indigotindisulfonate; Soluble indigo; Soluble indigo blue; Sumitomo Wool Blue SBC; Usacert Blue No. 2; Usacert FD and C Blue No. 2; WAS 35

CA Index Name 1H-Indole-5-sulfonic acid, 2-(1,3-dihydro-3-oxo-5-sulfo-2H-indol-2-ylidene)-2,3-dihydro-3-oxo-, disodium salt

CAS Registry Number 860-22-0

Merck Index Number 4944

Chemical Structure



Chemical/Dye Class Miscellaneous, Indigoid

Molecular Formula $C_{16}H_8N_2O_8S_2Na_2$

Molecular Weight 466.36

pH Range 11.5–14.0

Color Change at pH Blue (11.5) to yellow (14.0)

Physical Form Blue-purple powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 608 nm

Melting Point $>250^\circ\text{C}$

Synthesis Synthetic methods¹⁻⁹

Major Applications Display device,¹⁰ sensor,¹¹ chemical-mechanical polishing,¹² batteries,¹³ photographic materials,¹⁴ thermoplastics,¹⁵ inks,¹⁶ highlighters,¹⁷ detergents,¹⁸ disinfectants,¹⁹ rodenticide,²⁰ colored bubbles,²¹ hair dyes,²² cosmetics,²³ food,²⁴ determine bacterial growth,²⁵ antiischemic agents,²⁶ antiseptic,²⁷ antitumor agents,²⁸ Alzheimer's disease,²⁹ psychoactive drugs,³⁰ Tooth whitening,³¹ oral care agent³²

Safety/Toxicity Toxicity to reproductive system,³³ carcinogenicity,³⁴ cytotoxicity,³⁵ genotoxicity,³⁶ hypotension,³⁷ hypertension,³⁸ mutagenicity,³⁹ teratogenicity⁴⁰

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INDOPHENOL

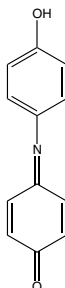
Other Names Indophenol; Benzenoneindophenol; Phenolindophenol

CA Index Name 2,5-Cyclohexadien-1-one, 4-[(4-hydroxyphenyl)imino]-

CAS Registry Number 500-85-6

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Miscellaneous

Molecular Formula C₁₂H₉NO₂

Molecular Weight 199.21

pH Range 6.3–12.3

Color Change at pH Red (6.3) to blue (12.3)

pKa 8.1, 9.4, 10.6

Physical Form Reddish-blue powder

Solubility Insoluble in water; soluble in ethanol

UV-Visible (λ_{max}) 602 nm

Melting Point >300°C

Boiling Point (Calcd.) 360.0 ± 42.0°C Pressure: 760 Torr

Synthesis Synthetic methods¹⁻³

Major Applications Liquid crystal display device,⁴ chemical-mechanical polishing,⁵ fuel cell,⁶ redox materials,⁷ hair dyes,⁸ lubricants,⁹ bacterial vaginosis screening technique,¹⁰ biosensor¹¹

Safety/Toxicity Environmental pollutants,¹² toxicity to fish¹³

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IODOPHENOL BLUE

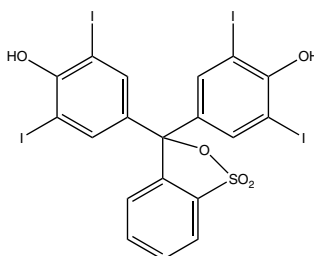
Other Names Iodophenol blue; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2,6-diiodo-, S,S-dioxide; 3H-2,1-Benzoxathiole, phenol deriv.; NSC 36792, Tetraiodophenolsulfonephthalein

CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2,6-diiodo-

CAS Registry Number 4430-24-4

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula C₁₉H₁₀I₄O₅S

Molecular Weight 857.96

pH Range 3.0–4.8

Color Change at pH yellow (3.0) to blue (4.8)

pKa 4.16

Physical Form Brown powder

Solubility Slightly soluble in water; soluble in ethanol, methanol, acetone, ether, acetic acid

UV-Visible (λ_{max}) 433 nm

Melting Point 229°C (decompose)

Boiling Point (Calcd.) 615.3 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic method¹

Major Applications Shelf life indicator,² determining proteins,³ human serum albumins,⁴ polymeric biguanides,⁵ examining renal and hepatic functions,⁶ apoptosis assay⁷

Safety/Toxicity No data available

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ISONITROSOTHIOCAMPHOR

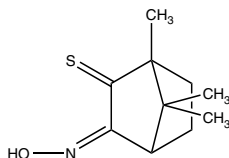
Other Names 2,3-Bornanedione, 2-thio-, 3-oxime; Isonitrosothiocamphor

CA Index Name Bicyclo[2.2.1]heptan-2-one, 4,7,7-trimethyl-3-thioxo-, oxime

CAS Registry Number 91156-63-7

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Miscellaneous

Molecular Formula C₁₀H₁₅NOS

Molecular Weight 197.30

pH Range 8.6–9.0

Color Change at pH Violet (8.6) to yellow (9.0)

pKa 9.42

Physical Form Violet crystals

Solubility Soluble in water, ethanol

Melting Point 148°C

Boiling Point (Calcd.) 292.1 ± 23.0°C Pressure: 760 Torr

Synthesis Synthetic method¹

Major Applications Reagent for rhodium,² platinum,³ cobalt,⁴ palladium,⁵ copper,⁶ cadmium,⁷ nickel⁸

Safety/Toxicity No data available

References

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ISOPICRAMIC ACID

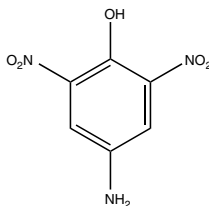
Other Names 4-Amino-2,6-dinitrophenol; Isopicramic acid

CA Index Name Phenol, 4-amino-2,6-dinitro-

CAS Registry Number 17973-92-1

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Nitro

Molecular Formula $C_6H_5N_3O_5$

Molecular Weight 199.12

pH Range 4.0–5.6

Color Change at pH Rose-pink (4.0) to yellow (5.6)

pKa 5.09

Physical Form Orange-brown powder

Solubility Insoluble in water; soluble in ethanol

Melting Point $>250^{\circ}\text{C}$

Boiling Point (Calcd.) $356.9 \pm 42.0^{\circ}\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Toys³

Safety/Toxicity No data available

References

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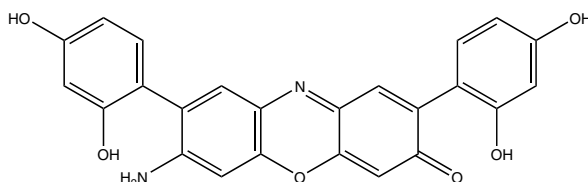
Other Names 2-Amino-3,6-bis(2,4-dihydroxyphenyl)-2-phenoxazone; Fluorescent Blue; Iris Blue B; Lacmoid; Resorcein; Resorcein Blue

CA Index Name 3H-Phenoxazin-3-one, 7-amino-2,8-bis(2,4-dihydroxyphenyl)-

CAS Registry Number 33869-21-5

Merck Index Number 5332

Chemical Structure



Chemical/Dye Class Miscellaneous

Molecular Formula C₂₄H₁₆N₂O₆

Molecular Weight 428.39

pH Range 4.4–6.4

Color Change at pH Red (4.4) to blue (6.4)

pKa 5.31

Physical Form Black-violet powder

Solubility Sparingly soluble in water, ether; soluble in water, ethanol, methanol, amyl alcohol, acetone, acetic acid; practically insoluble in chloroform, benzene, petroleum ether

UV-Visible (λ_{max}) 611 nm

Melting Point >250°C

Boiling Point (Calcd.) 755.3 ± 60.0°C Pressure: 760

Synthesis Synthetic methods^{1–3}

Major Applications Electrochromic devices,⁴ photosensitive materials,⁵ parasiticides,⁶ hair dyes,⁷ cosmetics,⁸ ointment for hemorrhoids⁹

Safety/Toxicity Fish toxicity¹⁰

References

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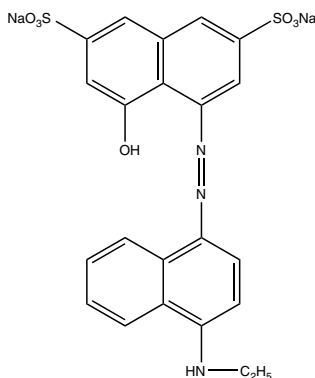
LANACYL VIOLET BF

Other Names 2,7-Naphthalenedisulfonic acid, 4-[[4-(ethylamino)-1-naphthyl]-azo]-5-hydroxy-, disodium salt; C.I. 13375; Lanacyl Violet BF

CA Index Name 2,7-Naphthalenedisulfonic acid, 4-[[4-(ethylamino)-1-naphthalenyl]azo]-5-hydroxy-, disodium salt

CAS Registry Number 10214-18-3

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Azo

Molecular Formula $C_{22}H_{17}N_3O_7S_2Na_2$

Molecular Weight 545.49

pH Range 11.0–13.0

Color Change at pH Violet (11.0) to orange (13.0)

pKa 12.12

Physical Form Solid

Solubility Soluble in water, ethanol

Melting Point >250°C

Synthesis No data available

Major Applications No data available

Safety/Toxicity No data available

Reference

No reference available

LUMINOL

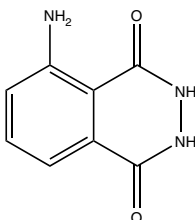
Other Names 3-Aminophthalhydrazide; 3-Aminophthalic acid hydrazide; 3-Aminophthalic hydrazide; 5-Amino-1,4-dihydroxyphthalazine; 5-Amino-2,3-dihydro-1,4-phthalazinedione; Luminol; NSC 5064

CA Index Name 1,4-Phthalazinedione, 5-amino-2,3-dihydro-

CAS Registry Number 521-31-3

Merck Index Number 5600

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula $C_8H_7N_3O_2$

Molecular Weight 177.16

pH Range 6.0–7.0

Color Change at pH Nonfluorescence (6.0) to blue fluorescence (7.0)

pKa (Calcd.) 10.50 ± 0.20 ;

0.58 ± 0.20

Physical Form Off-white to yellow powder

Solubility Insoluble in water, soluble in dimethyl sulfoxide, base

UV-Visible ($\lambda_{\max}$) 425 nm

Melting Point 319–320°C

Synthesis Synthetic methods^{1–12}

Major Applications Night vision devices,¹³ identification of product forgeries,¹⁴ determination of nitride in food,¹⁵ analytical chemistry,¹⁶ pharmaceuticals,¹⁷ iodine in biological materials,¹⁸ evaluating phagocytes,¹⁹ detecting tumors,²⁰ DNA,²¹ biosensors,^{22,23} assay of fungi,²⁴ bacteria,²⁴ yeasts,²⁴ assay of lipase activity²⁵

Safety/Toxicity *In vitro* biological effects,²⁶ cytotoxicity,²⁷ pulmonary toxicity,²⁸ mutagenicity,^{29,30} neurotoxicity³¹

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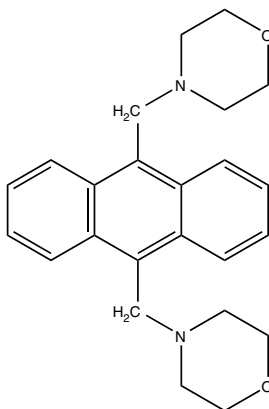
LYSOSENSOR BLUE DND 167

Other Names Morpholine, 4,4'-(9,10-anthrylenedimethylene)di-; LysoSensor Blue DND 167

CA Index Name Morpholine, 4,4'-[9,10-anthracenediylbis(methylene)]bis-

CAS Registry Number 101821-61-8

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Fluorescent

Molecular Formula C₂₄H₂₈N₂O₂

Molecular Weight 376.49

pH Range 4.5–6.0

Color Change at pH Strong blue fluorescence (4.5) to weak blue fluorescence (6.0)

pKa 5.1

Physical Form Solid

Solubility Insoluble in water; soluble in dimethyl sulfoxide

UV-Visible (λ_{max}) 373 nm

Melting Point >250°C

Boiling Point (Calcd.) 546.5 ± 45.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–3}

Major Applications Multifunctional reference system,⁴ pH probes for acidic organelles in living cells,⁵ methods for measuring & controlling multidrug resistance (MDR) of tumor cells,^{6,7} fluorescence lifetime characterization of lysosomal pH⁸

Safety/Toxicity No data available

References

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LYSOSENSOR BLUE DND 192

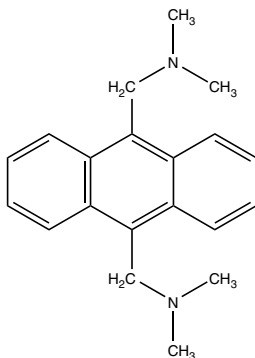
Other Names LysoSensor DND 192

CA Index Name 9,10-Anthracenedimethanamine, *N,N,N',N'*-tetramethyl-

CAS Registry Number 166821-89-2

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula C₂₀H₂₄N₂

Molecular Weight 292.42

pH Range 6.5–8.5

Color Change at pH Strong blue fluorescence (6.5) to weak blue fluorescence (8.5)

pKa 7.5

Physical Form Solid

Solubility Insoluble in water; Soluble in dimethyl sulfoxide

UV-Visible (λ_{max}) 374 nm

Melting Point >250°C

Boiling Point (Calcd.) 418.0 ± 25.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Fluorescence lifetime characterization of lysosomal pH³

Safety/Toxicity No data available

References

1. Tamayo, A.; Lodeiro, C.; Escriche, L.; Casabo, J.; Covelo, B.; Gonzalez, P. New fluorescence PET systems based on N₂S₂ pyridine-anthracene-containing macrocyclic ligands. spectrophotometric, spectrofluorimetric, and metal ion binding studies. *Inorg. Chem.* **2005**, *44*, 8105–8115.
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LYSOSENSOR GREEN DND 189

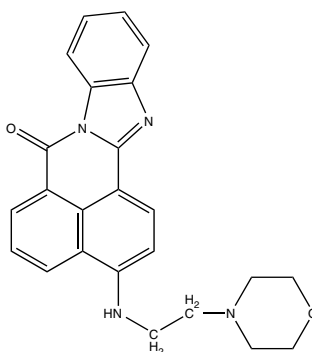
Other Names LysoSensor Green DND 189

CA Index Name 7H-Benzimidazo[2,1-a]benz[de]isoquinolin-7-one, 3-[[2-(4-morpholinyl)ethyl]amino]-

CAS Registry Number 152584-38-8

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula C₂₄H₂₂N₄O₂

Molecular Weight 398.46

pH Range 4.5–6.0

Color Change at pH Strong green fluorescence (4.5) to weak green fluorescence (6.0)

pKa 5.2

Physical Form Solid

Solubility Insoluble in water; soluble in dimethyl sulfoxide

UV-Visible (λ_{max}) 443 nm

Melting Point >250°C

Boiling Point (Calcd.) 704.9 ± 70.0°C Pressure: 760 Torr

Synthesis Synthetic methods¹

Major Applications Biosensors,² pH probes for acidic organelles in living cells,³ method for quantifying nucleic acid incorporated into target organelle,⁴ fluorescence lifetime characterization of lysosomal pH⁵

Safety/Toxicity No data available

References

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5. Lin, H.; Herman, P.; Kang, J. S.; Lakowicz, J. R. Fluorescence lifetime characterization of novel low-pH probes. *Anal. Biochem.* **2001**, 294, 118–125.

LYSOSENSOR YELLOW/BLE DND 160

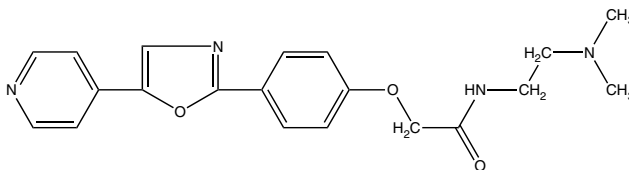
Other Names L 7545; Lyso Sensor DND 160; LysoSensor Yellow/Blue DND 160; PDMPO

CA Index Name Acetamide, *N*-[2-(dimethylamino)ethyl]-2-[4-[5-(4-pyridinyl)-2-oxazolyl]phenoxy]-

CAS Registry Number 231632-18-1

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula C₂₀H₂₂N₄O₃

Molecular Weight 366.41

pH Range 3.5–6.0

Color Change at pH Strong yellow-blue fluorescence (3.5) to weak yellow-blue fluorescence (6.0)

pKa 4.2

Physical Form Solid

Solubility Insoluble in water; soluble in dimethyl sulfoxide

UV-Visible (λ_{max}) 384 nm, 329 nm

Melting Point >250°C

Synthesis Synthetic methods^{1,2}

Major Applications Recording materials,³ biosensors,⁴ regulating acidity in gastric cells,⁵ for biological silicification studies,¹ fluorescence lifetime characterization of lysosomal pH²

Safety/Toxicity No data available

References

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M

MAGDALA RED

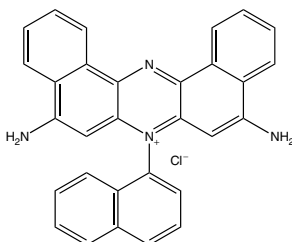
Other Names Dibenzo[a,j]phenazinium, 5,9-diamino-7-(1-naphthyl)-, chloride; Magdala Red; Magdaline red; Magdalskaya red

CA Index Name Dibenzo[a,j]phenazinium, 5,9-diamino-7-(1-naphthalenyl)-, chloride

CAS Registry Number 10114-42-8

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula $C_{30}H_{21}N_4Cl$

Molecular Weight 472.96

pH Range 3.0–4.0

Color Change at pH Nonfluorescence (3.0) to purple fluorescence (4.0)

Physical Form Dark brown powder or green needles

Solubility Sparingly soluble in hot water; soluble in ethanol

Melting Point >250°C

Synthesis Synthetic methods¹

Major Applications Display device,² inks,³ optical materials,⁴ determination of proteins,⁵ nucleic acid,⁶ clay minerals⁷

Safety/Toxicity No data available

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MALACHITE GREEN

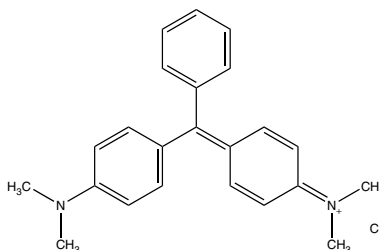
Other Names C.I. Basic Green 4; Victoria Green WB; ADC Malachite Green Crystals; Acryl Brilliant Green B; Aizen Malachite Green; Aizen Malachite Green Crystals; Aizen malachite green liquid; Aniline green; Astra Malachite Green; Astra Malachite Green B; Astra Malachite Green BXX; Atlantic Malachite Green; Basacryl Green X-BF; Basic Green 4; Basonyl Green 830; Basonyl Green NB 832; Benzal Green; Benzaldehyde green; Bronze Green Toner A 8002; Burma Green B; C.I. 42000; Calcozine Green V; China Green; Diabasic Malachite Green; Diamond Green B extra; Diamond Green BX; Diamond Green P Extra; Green MX; Green Malaquite; Grenoble Green; Hidaco Malachite Green Base; Hidaco Malachite Green LC; Hidaco Malachite Green SC; LC 6220; Light Green N; Lincoln Green Toner B 15-2900; Malachite Green 4; Malachite Green A; Malachite Green AN; Malachite Green B; Malachite Green CP; Malachite Green Crystals; Malachite Green Crystals BPC; Malachite Green J 3E; Malachite Green Powder; Malachite Green WS; Malachite Green XLS; Malachite Lake Green A; Malachite green; Malachite green chloride; Mitsui Malachite Green; New Victoria Green Extra I; New Victoria Green Extra II; New Victoria Green Extra O; Oji Malachite Green; Solid Green Crystals O; Solid Green O; Super Ick Cure; Tertrophen Green M; Tokyo Aniline Malachite Green; Verona Basic Green M; Victoria Green; Victoria Green (basic dye); Victoria Green B; Victoria Green S; Victoria Green WPB

CA Index Name Methanaminium, *N*-[4-[[4-(dimethylamino)phenyl]-phenylmethylene]-2,5-cyclohexadien-1-ylidene]-*N*-methyl-, chloride

CAS Registry Number 569-64-2

Merck Index Number 5699

Chemical Structure



Chemical/Dye Class Triphenylmethane

Molecular Formula $C_{23}H_{25}N_2Cl$

Molecular Weight 364.92

pH Range 0.0–2.0;

11.6–14.0

Color Change at pH Yellow (0.0) to green (2.0)

Green (11.6) to colorless (14.0)

pKa 6.90

Physical Form Green crystals

Solubility Very soluble in water; soluble in ethanol, methanol, amyl alcohol

UV-Visible (λ_{max}) 615 nm, 425 nm

Melting Point 112–114°C

Synthesis Synthetic methods^{1–13}

Major Applications Photoresists,¹⁴ color filter,¹⁵ printed circuit board,¹⁶ sol-gel matrix,¹⁷ liquid crystal displays,¹⁸ decoder system,¹⁹ inks,²⁰ highlighters,²¹ herbicides,²² disinfectants,²³ cosmetics,²⁵ identifying mammal genes,²⁵ detecting nucleic acids,²⁶ mycobacterial growth,²⁷ multidrug resistance inhibitors,²⁸ radiochemotherapy,²⁹ wound dressing materials,³⁰ antitumor agents,³¹ treatment of patients with pulmonary tuberculosis³²

Safety/Toxicity Acute toxicity,³³ carcinogenicity,³⁴ cytotoxicity,³⁵ genotoxicity,³⁶ mutagenicity,³⁷ toxicological effects³⁸

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MARTIUS YELLOW

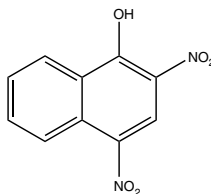
Other Names Acid Yellow 24; 1-Naphthol, 2,4-dinitro-; 1-Hydroxy-2,4-dinitronaphthalene; 2,4-Dinitro-1-naphthol; 2,4-Dinitronaphthol; Martinsgelb; Martius yellow; Manchester Yellow; NSC 6148

CA Index Name 1-Naphthalenol, 2,4-dinitro-

CAS Registry Number 605-69-6

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Nitro

Molecular Formula C₁₀H₆N₂O₅

Molecular Weight 234.16

pH Range 2.0–3.2

Color Change at pH Colorless (2.0) to yellow (3.2)

pKa 2.12

Physical Form Yellow orange powder

Solubility Very slightly soluble in water, ethanol

UV-Visible (λ_{max}) 430 nm, 420 nm, 432 nm

Melting Point 138°C

Boiling Point (Calcd.) 407.9 ± 35.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–11}

Major Applications Photoresists,¹² magnetic recording materials,¹³ explosives,¹⁴ polymerization inhibitor,¹⁵ surface coatings,¹⁶ coloring hair,¹⁷ for animal identification¹⁸

Safety/Toxicity Toxicology,¹⁹ toxicity,^{20,21} mutagenicity^{22,23}

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MESALAMINE

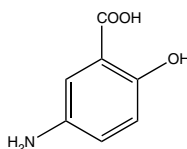
Other Names Salicylic acid, 5-amino-; 2-Hydroxy-5-aminobenzoic acid; 3-Carboxy-4-hydroxy-aniline; 5-ASA; 5-Amino-2-hydroxybenzoic acid; 5-Aminosalicylic acid; Asacol; Asacolitin; Asacolon; Canasa; Claversal; Fisalamine; Ipocol; Lixacol; Mesacol; Mesalamine; Mesalazine; Mesasal; NSC 38877; Pentasa; Rowasa; Salofalk; Salozinal; *m*-Aminosalicylic acid

CA Index Name Benzoic acid, 5-amino-2-hydroxy-

CAS Registry Number 89-57-6

Merck Index Number 5904

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula C₇H₇NO₃

Molecular Weight 153.14

pH Range 3.1–4.4

Color Change at pH Nonfluorescence (3.1) to light green fluorescence (4.4)

pKa 2.74, 5.84

Physical Form White to pinkish crystals

Solubility Slightly soluble in cold water, ethanol; more soluble in hot water; soluble in hydrochloric acid

Melting Point 280°C (decompose)

Boiling Point (Calcd.) 403.9 ± 40.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–14}

Major Applications Detergent,¹⁵ hair dyes,¹⁶ prevention of colorectal cancer,¹⁷ treating inflammatory bowel disease,¹⁸ autoimmune disorders,¹⁹ gastrointestinal inflammation,²⁰ chemokine-mediated diseases,²¹ mucosal tissue disorder,²² sleep disorders,²³ rectoanal tenesmus,²⁴ ulcerative colitis²⁵

Safety/Toxicity Hepatotoxicity,^{26,27} cytotoxicity,^{27,28} nephrototoxicity,²⁹ risk of renal disease,³⁰ safety in pregnancy,³¹ side effects³²

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METANIL YELLOW

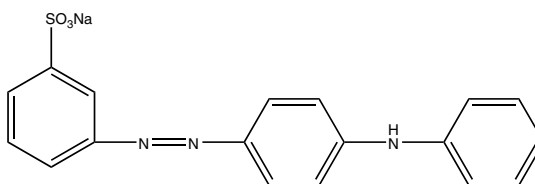
Other Names Benzenesulfonic acid, *m*-(*p*-anilinophenylazo)-, sodium salt; C.I. Acid Yellow 36; C.I. Acid Yellow 36, monosodium salt; 11363 Yellow; Acid Gold Yellow G; Acid Golden G; Acid Golden Yellow G; Acid Leather Yellow PRW; Acid Leather Yellow R; Acid Yellow 36; Acid Yellow Metanil; Aizen Metanil Yellow; Amacid Yellow M; Basacid Yellow 230; Basacid Yellow 232; Brasilan Metanil Yellow; Bucacid Metanil Yellow; C Ext. Yellow 10; C.I. 13065; Calcocid Yellow MXXX; Diacid Metanil Yellow; Egacid Yellow M; Egacid Yellow MA; Eniacid Metanil Yellow GN; Ext D & C Yellow 1; Ext D and C Yellow No. 1; Fenazo Yellow M; Hidacid Metanil Yellow; Hispacid Yellow MG; Japan Yellow 406; Japan Yellow No. 406; Java Metanil Yellow G; Kiton Orange MNO; Kiton Yellow MS; Metanil Yellow; Metanil Yellow 1955; Metanil Yellow C; Metanil Yellow E; Metanil Yellow Extra; Metanil Yellow F; Metanil Yellow G; Metanil Yellow Griesbach; Metanil Yellow K; Metanil Yellow KRSU; Metanil Yellow M; Metanil Yellow M 3X; Metanil Yellow O; Metanil Yellow PL; Metanil Yellow S; Metanil Yellow Supra P; Metanil Yellow VS; Metanil Yellow WS; Metanil Yellow Y; Metanil Yellow YK; Metanile Yellow O; Metanilic Yellow; Mitsui Metanil Yellow; Remaderm Yellow HPR; Shikiso Metanil Yellow; Sodium 4'-anilinoazobenzene-3-sulfonate; Sodium *m*-(4-anilinophenylazo)-benzenesulfonate; Sodium *m*-sulfonate-*p*-phenylazodiphenylamine; Symulon Metanil Yellow; Takaoka Metanil Yellow; Tertracid Yellow M; Tropaeolin G; Vondacid Metanil Yellow G; Yellow Methanil; Yellow No. 406; Yodochrome Metanil Yellow

CA Index Name Benzenesulfonic acid, 3-[[4-(phenylamino)phenyl]azo]-, monosodium salt

CAS Registry Number 587-98-4

Merck Index Number 5928

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula C₁₈H₁₄N₃O₃SNa

Molecular Weight 375.38

pH Range 1.2–2.3

Color Change at pH Red (1.2) to yellow (2.3)

Physical Form Orange-red powder

Solubility Soluble in water, ethanol; moderately soluble in ether, benzene; slightly soluble in acetone, xylene

UV-Visible (λ_{max}) 414 nm, 435 nm

Melting Point >250°C

Synthesis Synthetic methods¹

Major Applications Display device,² nanoparticles,³ optical sensors,⁴ batteries,⁵ lithographic printing plates,⁶ inks,⁷ highlighters,⁸ children's coloring books,⁹ floor coatings,¹⁰ disinfectants,¹¹ hair dyes,^{12–14} personal care products,¹⁵ cosmetics,¹⁶ food storage,¹⁷ antiseptic,¹⁸ dental impression materials¹⁹

Safety/Toxicity Acute toxicity,²⁰ carcinogenic effects,²¹ hepatocarcinogenesis,²² mutagenicity^{23,24}

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2-METHOXYBENZALDEHYDE

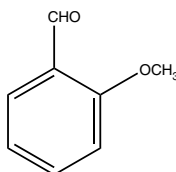
Other Names Benzaldehyde, *o*-methoxy-; *o*-Anisaldehyde; 2-Anisaldehyde; 2-Methoxybenzaldehyde; 2-Methoxybenzenecarboxaldehyde; 2-Methoxyphenylformaldehyde; 6-Methoxybenzaldehyde; NC 064; NSC 58960; Salicylaldehyde methyl ether; *o*-Formylanisole; *o*-Methoxybenzaldehyde

CA Index Name Benzaldehyde, 2-methoxy-

CAS Registry Number 135-02-4

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula C₈H₈O₂

Molecular Weight 136.15

pH Range 3.1–4.4

Color Change at pH Nonfluorescence (3.1) to green fluorescence (4.4)

Physical Form Off-white to light yellow crystals

Solubility Slightly soluble in water; soluble in ethanol

Melting Point 37–39°C

Boiling Point 238°C

Synthesis Synthetic methods^{1–6}

Major Applications Battery,^{7,8} hair dyes,^{9,10} bird repellents,^{11,12} cosmetics,¹³ antibacterial,¹⁴ anti-pyretic agent¹⁵

Safety/Toxicity Aquatic toxicity,¹⁶ algae toxicity¹⁷

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4-METHYLESCULETIN

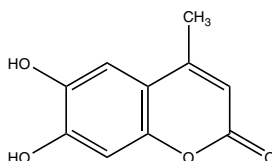
Other Names Coumarin, 6,7-dihydroxy-4-methyl-; Esculetin, 4-methyl-; 4-Methyl-6,7-dihydroxy-coumarin; 4-Methylaesculetin; 4-Methylesculetin; 4-Methylesculetol; 6,7-Dihydroxy-4-methyl-coumarin; Methylesculetin; NSC 11828; NSC 688807

CA Index Name 2H-1-Benzopyran-2-one, 6,7-dihydroxy-4-methyl-

CAS Registry Number 529-84-0

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Coumarin

Molecular Formula C₁₀H₈O₄

Molecular Weight 192.17

pH Range 4.0–6.2

Color Change at pH Colorless (4.0) to blue fluorescent (6.2)

pKa 8.72

Physical Form Light brown powder

Solubility Very slightly soluble in water; slightly soluble in ethanol; soluble in ether, chloroform, ethylene glycol

UV-Visible ($\lambda_{\max}$) 348 nm, 292 nm

Melting Point 274–276°C

Boiling Point (Calcd.) 455.5 ± 45.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–9}

Major Applications Electroluminescent device,¹⁰ photoresists,^{11,12} photography,^{13,14} analytical reagent,¹⁵ cosmetics,^{16–19} hair dye,^{20–29} shampoo,^{30,31} antioxidant,³² hypotensive agent,³³ antiinflammatory agent,³⁴ antiviral agent,³⁵ multidrug resistance (MDR) modulator,³⁶ inhibitory effect on melanin biosynthesis,³⁷ protective agent against DNA damage,³⁸ antimutagenic agent,^{39–41} detection of tumor cell-specific cytotoxicity,⁴² antiproliferative agent against cancer cells,⁴³ analysis of human pancreatic cancer cell activity,⁴⁴ chondroprotective agent⁴⁵

Safety/Toxicity Chondroprotective agent⁴⁵

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METHYL GREEN

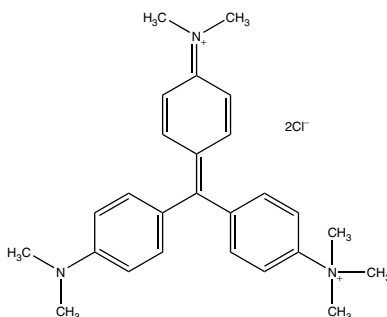
Other Names Methyl Green

CA Index Name Methyl Green

CAS Registry Number 54327-10-5

Merck Index Number Not listed

Chemical Structure



Note: The traditional Methyl Green has not manufactured for decades. The dye sold as Methyl Green is more accurately described as Ethyl Green. Both, Methyl Green and Ethyl Green are sold as double zinc salts.

Chemical/Dye Class Triphenylmethane

Molecular Formula $C_{26}H_{33}N_3Cl_2$

Molecular Weight 458.46

pH Range 0.1–2.3

Color Change at pH Yellow (0.1) to greenish-blue (2.3)

Physical Form Green crystalline power

Solubility Soluble in water, ethanol; insoluble in xylene

UV-Visible (λ_{max}) 635 nm, 420 nm

Melting Point >300°C

Synthesis Synthetic methods^{1,2}

Major Applications Liquid crystal display device,³ photography,⁴ recording materials,⁵ inks,⁶ cosmetics,⁷ DNA staining,⁸ cancer detection⁹

Safety/Toxicity Toxicity to fresh water organisms¹⁰

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METHYL ORANGE

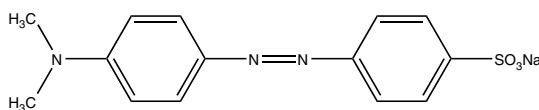
Other Names Benzenesulfonic acid, *p*-[[*p*-(dimethylamino)phenyl]azo]-, sodium salt; Orange III; 4-Dimethylaminoazobenzene-4'-sulfonic acid sodium salt; C.I. 13025; C.I. Acid Orange 52; Diazo-ben; Eniamethyl Orange; Gold orange; Helianthine; Helianthine B; KCA Methyl Orange; Methyl Orange B; Methyl orange; Orange 3; Sodium 4'-(dimethylamino)azobenzene-4-sulfonate; Sodium 4-(dimethylamino)azobenzene-4'-sulfonate; Sodium 4-[4-(dimethylamino)-phenylazo]-benzene-sulfonate; Sodium *p*-[*p*-(dimethylamino)-phenylazo]-benzenesulfonate; Sodium *p*-dimethylaminoazobenzenesulfonate; Tropaeolin D

CA Index Name Benzenesulfonic acid, 4-[[4-(dimethylamino)phenyl]azo]-, sodium salt

CAS Registry Number 547-58-0

Merck Index Number 6105

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula C₁₄H₁₄N₃O₃SNa

Molecular Weight 327.34

pH Range 3.0–4.4

Color Change at pH Red (3.0) to yellow (4.4)

pKa 3.76, 3.40

Physical Form Orange powder

Solubility Slightly soluble in water, more soluble in hot water; practically insoluble in ethanol

UV-Visible (λ_{max}) 507 nm, 522 nm, 464 nm

Melting Point >300°C

Synthesis Synthetic methods^{1–9}

Major Applications Liquid crystals,¹⁰ thin films,¹¹ sensors,¹² sol-gel matrix,¹³ waveguides,¹⁴ host-guest chemistry,¹⁵ display device,¹⁶ corrosion inhibitor,¹⁷ glass coatings,¹⁸ paints,¹⁹ wound dressing materials,²⁰ pharmaceuticals,²¹ dental materials,²² measuring nucleic acid²³

Safety/Toxicity Carcinogenicity,²⁴ genotoxicity,²⁵ mutagenicity²⁶

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METHYL PURPLE

Other Names Fleisher's Methyl purple indicator

CA Index Name Methyl purple

CAS Registry Number 1340-02-9

Merck Index Number Not listed

Chemical Structure No structure diagram available

Chemical/Dye Class No data available

Molecular Formula Unspecified

Molecular Weight No data available

pH Range 4.8–5.4

Color Change at pH Purple (4.8) to green (5.4)

pKa No data available

Physical Form Green powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 410 nm, 620 nm

Melting Point Not available

Synthesis Synthetic method¹

Major Applications Analysis of selenium in marine organisms,^{2,3} detecting lactic acid bacteria,⁴ determination of iron in human hair,⁵ antimicrobial agent⁶

Safety/Toxicity No data available

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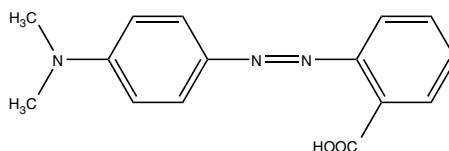
METHYL RED

Other Names C.I. Acid Red 2; 2-Carboxy-4'-(dimethylamino)azobenzene; 2-[(*p*-Dimethylamino)-phenyl]azobenzoic acid; 2-[[4-(Dimethylamino)-phenyl]azo]benzoic acid; 4'-(Dimethylamino)-azobenzene-2-carboxylic acid; 4-(2-Carboxyphenylazo)-*N,N*-dimethylaniline; Acid Red 2; C.I. 13020; Methyl red; Methyl red C.I. 13020; NSC 215212; NSC 34729; NSC 9597; *o*-Methyl red; *o*-[[*p*-(Dimethylamino)-phenyl]azo]-benzoic acid; *p*-(Dimethylamino)-azobenzene-*o*-carboxylic acid

CA Index Name Benzoic acid, 2-[[4-(dimethylamino)phenyl]azo]-

CAS Registry Number 493-52-7

Merck Index Number 6119

Chemical Structure

Chemical/Dye Class Azo

Molecular Formula C₁₅H₁₅N₃O₂

Molecular Weight 269.30

pH Range 4.4–6.2

Color Change at pH Red (4.4) to yellow (6.2)

pKa 5.06, 2.3, 2.5, 4.95

Physical Form Maroon-red crystals

Solubility Almost insoluble in water; soluble in ethanol, acetic acid

UV-Visible (λ_{max}) 410 nm, 530 nm, 427 nm, 519 nm

Melting Point 181–182°C

Boiling Point (Calcd.) 479.5 ± 30.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–4}

Major Applications Waveguides,⁵ LED sensors,⁶ photoresists,⁷ liquid crystals,⁸ sol-gel matrix,⁹ optical sensors,¹⁰ paints,¹¹ toys,¹² detection of thiols,¹³ food freshness sensors,¹⁴ dental product,¹⁵ saliva sampling method,¹⁶ detecting lactic acid,¹⁷ carbohydrates¹⁸

Safety/Toxicity Carcinogenicity,¹⁹ genotoxicity,²⁰ mutagenicity²¹

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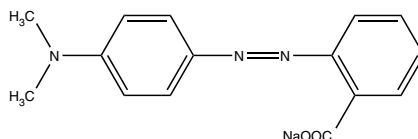
METHYL RED, SODIUM SALT

Other Names C.I. Acid Red 2, sodium salt; Methyl red sodium salt; *o*-Methyl red sodium salt

CA Index Name Benzoic acid, 2-[[4-(dimethylamino)phenyl]azo]-, sodium salt

CAS Registry Number 845-10-3

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Azo

Molecular Formula C₁₅H₁₄N₃O₂Na

Molecular Weight 291.29

pH Range 1.2–3.4;

4.2–6.3

Color Change at pH Red (1.2) to orange (3.4)

Red (4.2) to yellow (6.3)

pKa 2.3, 5.0

Physical Form Orange powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 437 nm, 410 nm, 493 nm

Melting Point >300°C

Synthesis Synthetic methods^{1,2}

Major Applications Optical filters,^{3,4} liquid crystal cells,^{5,6} holography,^{7,8} inks,⁹ toner,¹⁰ corrosion inhibitor,¹¹ detergent¹²

Safety/Toxicity No data available

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4-METHYUMBELLIFERONE

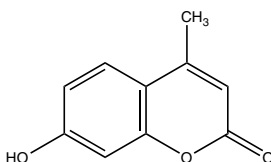
Other Names Coumarin, 7-hydroxy-4-methyl-; Umbelliferone, 4-methyl-; β -Methylumbelliferone; 4-MU; 4-Methyl-7-hydroxycoumarin; 4-Methylumbelliferone; 7-Hydroxy-4-methyl-2-chromenone; 7-Hydroxy-4-methyl-2-oxo-3-chromene; 7-Hydroxy-4-methyl-2H-1-benzopyran-2-one; 7-Hydroxy-4-methyl-2H-chromen-2-one; 7-Hydroxy-4-methylcoumarin; Bilcolic; Bilicante; Biliton H; Cantabilin; Cantabiline; Cholestil; Cholonerton; Cholspasmin; Coumarin 4; Coumarin 456; Cumarote C; Eurogale; Himecol; Hymecromone; Imecromone; LM 94; Medilla; Mendiaxon; NSC 19026; NSC 9408; Omega 127; Pilot 447

CA Index Name 2H-1-Benzopyran-2-one, 7-hydroxy-4-methyl-

CAS Registry Number 90-33-5

Merck Index Number 4854

Chemical Structure



Chemical/Dye Class Fluorescent, Coumarin

Molecular Formula $C_{10}H_8O_3$

Molecular Weight 176.17

pH Range 0.0–2.0;

6.5–8.0

Color Change at pH Green fluorescent (0.0) to weak blue fluorescent (2.0)

Weak blue fluorescent (6.5) blue fluorescent (8.0)

pKa 7.79

Physical Form White to off-white powder

Solubility Practically insoluble in water; slightly soluble in ethanol, ether, chloroform; soluble in methanol

UV-Visible ($\lambda_{\max}$) 221 nm, 251 nm, 322 nm

Melting Point 194–195°C

Boiling Point (Calcd.) $377.4 \pm 37.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods^{1–15}

Major Applications Color filter,¹⁶ electroluminescent displays,¹⁷ document security processes,¹⁸ lasers,¹⁹ integrated circuits,²⁰ liquid crystal displays,²¹ surface brightening composition,²² oil products,²³ teeth whitening agent,²⁴ lysosomal enzyme assay,²⁵ substrate for lipase,²⁶ determining protein-protein-interactions in living cells,²⁷ Antitrypanosomal,²⁸ antileishmanial,²⁸ anticancer,²⁹ antiHIV,³⁰ antimalarial,³¹ antibacterial,³² antifungal³²

Safety/Toxicity Acute oral toxicity,³³ ecotoxicology,³⁴ human health effects,³⁵ mutagenicity³⁶

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METHYL VIOLET

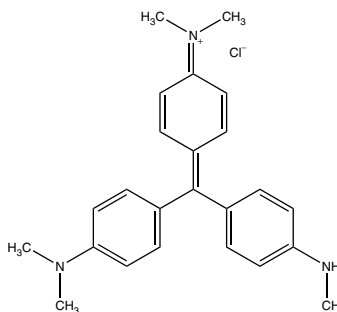
Other Names Methyl Violet; Aizen Methyl Violet BB; Aizen Methyl Violet Pure Special; Basic Violet 1; Basic Violet 5BN; Basic Violet K; Basonyl Violet 600; C Ext. Violet 5; C.I. 42535; Gentian Violet B; Methyl Violet 2B; Methyl Violet 6B; Methyl Violet B; Methyl Violet BB; Methyl Violet FN; Methyl Violet N; Methyl Violet Pure Special; Methyl Violet pure SP; Paris Violet R; Pyoktanin blue; Pyoktaninum coeruleum; Violet Powder H 2503

CA Index Name C.I. Basic Violet 1

CAS Registry Number 8004-87-3

Merck Index Number Not listed

Chemical Structure It is a mixture of *N*-pentamethyl (as shown) and *N*-hexamethyl (which is Crystal Violet) *p*-rosaniline chlorides



Chemical/Dye Class Triphenylmethane

Molecular Formula Mixture of tetra-, penta-, & hexamethyl *p*-rosaniline chlorides

Molecular Weight Mixture of tetra-, penta-, & hexamethyl *p*-rosaniline chlorides

pH Range 0.15–3.2

Color Change at pH Yellow (0.15) to violet (3.2)

Physical Form Green crystals

Solubility Soluble in water, ethanol, chloroform; insoluble in ether, xylene

UV-Visible (λ_{max}) 584 nm

Melting Point 137°C (decompose)

Synthesis Synthetic methods^{1–6}

Major Applications Display device,^{7,8} photoresists,⁹ solar cells,¹⁰ inks,^{11,12} highlighters,¹³ rubber,¹⁴ lithium battery,¹⁵ petroleum products,¹⁶ leak detection method,¹⁷ decoder system,¹⁸ packaging materials,¹⁹ hair dyes,²⁰ cosmetics,²¹ wound dressing materials,²² antitumor agent,²³ determination of nucleic acids²⁴

Safety/Toxicity Acute toxicity,²⁵ carcinogenicity,²⁶ toxicity to aquatic microbes,²⁷ mutagenicity²⁸

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METHYL YELLOW

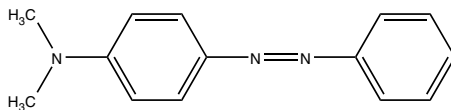
Other Names Aniline, *N,N*-dimethyl-*p*-phenylazo-; Butter yellow; C.I. Solvent Yellow 2; (4-Dimethylaminophenyl)phenyldiazene; (*p*-Dimethylaminophenyl)phenyldiazene; 4-(Dimethylamino)-azobenzene; 4-(*N,N*-Dimethylamino)azobenzene; 4-(Phenylazo)-*N,N*-dimethylaniline; Brilliant Fast Oil Yellow; Brilliant Fast Spirit Yellow; Brilliant Oil Yellow; C.I. 11020; Cerasine Yellow GG; DAB; DAB (carcinogen); DMAB; Dimethyl Yellow; Enial Yellow 2G; Fast Oil Yellow B; Fat Yellow; Fat Yellow A; Fat Yellow AD OO; Fat Yellow ES; Fat Yellow ES Extra; Fat Yellow R; Fat Yellow extra conc; Grasal Brilliant Yellow; Iketon Yellow Extra; Methyl yellow; *N,N*-Dimethyl-4-(phenylazo)aniline; *N,N*-Dimethyl-*p*-(phenylazo)aniline; NSC 6236; Oil Yellow 20; Oil Yellow 2625; Oil Yellow 2G; Oil Yellow BB; Oil Yellow D; Oil Yellow FN; Oil Yellow G; Oil Yellow GG; Oil Yellow GR; Oil Yellow II; Oil Yellow N; Oil Yellow PEL; Oil Yellow S; Oleal Yellow 2G; Organol Yellow ADM; Orient Oil Yellow GG; Petrol Yellow WT; Resinol Yellow GR; Silotras Yellow T 2G; Somalia Yellow A; Stear Yellow JB; Sudan Yellow GG; Sudan Yellow GGA; Toyo Oil Yellow G; Waxoline Yellow ADS; Yellow G Soluble in Grease; *p*-(Dimethylamino)azobenzene

CA Index Name Benzenamine, *N,N*-dimethyl-4-(phenylazo)-

CAS Registry Number 60-11-7

Merck Index Number 3229

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula $C_{14}H_{15}N_3$

Molecular Weight 225.29

pH Range 2.9-4.0

Color Change at pH Red (2.9) to yellow (4.0)

pKa 3.3, 3.4

Physical Form Orange-yellow powder

Solubility Insoluble in water; soluble in ethanol, benzene, ether, chloroform, petroleum ether, mineral acids, oils

UV-Visible ($\lambda_{\max}$) 408 nm, 256 nm, 508 nm

Melting Point 114–117°C

Boiling Point (Calcd.) $371.1 \pm 25.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods¹⁻⁸

Major Applications Electrochromic materials,⁹ sol-gel coatings,¹⁰ display device,¹¹ inks,¹² gas detection apparatus,¹³ nematocides,¹⁴ hair dyes,¹⁵ diapers,¹⁶ food storage,¹⁷ status assessment in breast cancer,¹⁸ detecting carbohydrates,¹⁹ bacteria,²⁰ diagnosing cervical disease,²¹ wound dressing materials²²

Safety/Toxicity Cytotoxicity,²³ carcinogenicity,²⁴ mutagenicity²⁵

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N

α -NAPHTHOIC ACID

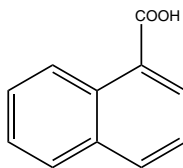
Other Names 1-Naphthoic acid; α -Naphthoic acid; α -Naphthylcarboxylic acid; 1-Carboxynaphthalene; 1-Naphthylcarboxylic acid; NSC 37569; Naphthalene- α -carboxylic acid

CA Index Name 1-Naphthalenecarboxylic acid

CAS Registry Number 86-55-5

Merck Index Number 6381

Chemical Structure



Chemical/Dye Class Fluorescent, Naphthalene

Molecular Formula $C_{11}H_8O_2$

Molecular Weight 172.18

pH Range 2.5–3.5

Color Change at pH Nonfluorescence (2.5) to blue fluorescence (3.5)

pKa 3.68

Physical Form Colorless crystals

Solubility Slightly soluble in hot water; freely soluble in hot ethanol, ether

UV-Visible ($\lambda_{\max}$) 293 nm

Melting Point 161°C

Boiling Point 300°C

Synthesis Synthetic methods^{1–13}

Major Applications Photoresists,¹⁴ recording materials,¹⁵ waveguides,¹⁶ battery,¹⁷ ink,¹⁸ rubber,^{19,20} plastic films,²¹ agriculture,²² cosmetics,²³ sunscreens,²⁴ method for preserving food,²⁵ drugs,²⁶ biosensors²⁷

Safety/Toxicity Acute toxicity,²⁸ skin corrosivity²⁹

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β -NAPHTHOL

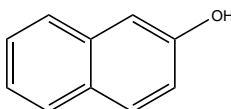
Other Names 2-Naphthol; β -Hydroxynaphthalene; β -Naphthol; β -Naphthyl alcohol; 2-Hydroxynaphthalene; Azogen Developer A; Betanaphthol; C.I. 37500; C.I. Azoic Coupling Component 1; C.I. Developer 5; Developer A; Developer AMS; Developer BN; Developer NA; Isonaphthol; NSC 2044; NSC 5737; Naphthol B

CA Index Name 2-Naphthalenol

CAS Registry Number 135-19-3

Merck Index Number 6384

Chemical Structure



Chemical/Dye Class Fluorescent, Naphthalene

Molecular Formula $C_{10}H_8O$

Molecular Weight 144.17

pH Range 8.5–9.5

Color Change at pH Nonfluorescence (8.5) to blue fluorescence (9.5)

pKa 9.57

Physical Form Buff crystals

Solubility Very slightly soluble in water; soluble in ethanol, ether, glycerin

UV-Visible (λ_{max}) 226 nm, 265 nm, 275 nm, 286 nm, 320 nm, 331 nm

Melting Point 120–123°C

Boiling Point 285–286°C

Synthesis Synthetic methods^{1–13}

Major Applications Display device,¹⁴ semiconductors,¹⁵ photoimaging materials,¹⁶ inks,¹⁷ toner,¹⁸ chalk,¹⁹ security paper,²⁰ molding materials,²¹ tin plating method,²² rubber,²³ adhesive,²⁴ leather,²⁵ detergent,²⁶ hair dyes,²⁷ antimitotic drug,²⁸ anticancer agent,²⁹ antiinflammatory agent,³⁰ treatment of acne vulgaris (pimples)³¹ and other dermal ailments (rashes, scratches, blemishes, hair loss),³¹ neurological disorders³²

Safety/Toxicity Acute toxicity,³³ skin corrosivity,³⁴ cytotoxicity,³⁵ carcinogenicity,³⁶ aquatic toxicity,³⁷ ecotoxicity,³⁸ immunotoxicity,³⁹ environmental toxicity,⁴⁰ mutagenicity,⁴¹ phytotoxicity⁴²

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NAPHTHOL AS

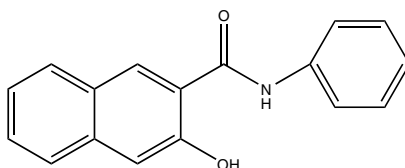
Other Names 2-Naphthanilide, 3-hydroxy-; α -Naphthol AS; 2-Hydroxy-3-(phenylcarbamoyl)naphthalene; 2-Hydroxy-3-naphthalenecarboxanilide; 2-Hydroxy-3-naphthanilide; 2-Hydroxy-3-naphthoic acid anilide; 2-Hydroxy-3-naphthoic anilide; 2-Hydroxy-N-phenyl-3-naphthalenecarboxamide; 2-Naphthol-3-carboxylic acid N-phenylamide; 3-(N-Phenylcarbamoyl)-2-naphthol; 3-Hydroxy-2-naphthalenecarboxanilide; 3-Hydroxy-2-naphthanilide; 3-Hydroxy-2-naphthoic acid anilide; 3-Hydroxy-N-phenyl-2-naphthalenecarboxamide; 3-Hydroxy-N-phenyl-2-naphthamide; 3-Hydroxyl-2-naphthanilide; Acco Naphthol AS; Acna Naphthol C; Amanil Naphthol AS; Amarthol AS; Anthonaphthol AS; Aquafine Red E 9; Azoground AS; Azoic Coupling Component 2; Azonaphtol A; Azotol A; Brenthol AS; C.I. 37505; C.I. Azoic Coupling Component 2; Celcot RF; Cibanaphthol RF; Diathol AS; Diathol ASF; Dragonthol A; Hiltonaphthol AS; Kako Grounder AS; Kambothol AS; Lake Developer A; Mitsui Naphthozol AS; N-Phenyl-2-hydroxy-3-naphthalenecarboxamide; NSC 45173; Naftolo MM; Naphtanilide OL Supra; Naphtanilide RC; Naphtanilide RC Supra; Naphtazol A; Naphthanil AS; Naphthoide AS; Naphthoide AS No. 100; Naphthol ACNA C; Naphthol AS; Naphthol AS Supra; Naphthol AS-A; Naphtholate AS; Naphtoelan A; Naphtol AS; Solunaphtol A; Tulathol AS; Ultrazol I-AS

CA Index Name 2-Naphthalenecarboxamide, 3-hydroxy-*N*-phenyl-

CAS Registry Number 92-77-3

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Naphthalene

Molecular Formula $C_{17}H_{13}NO_2$

Molecular Weight 263.29

pH Range 8.2–10.3

Color Change at pH Nonfluorescence (8.2) to yellow/green fluorescence (10.3)

pKa 9.70

Physical Form Beige powder

Solubility Insoluble in water; sparingly soluble in ethanol

UV-Visible ($\lambda_{\max}$) 394 nm

Melting Point 247–250°C

Boiling Point (Calcd.) $391.8 \pm 25.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods^{1–11}

Major Applications Sensors,¹² recording materials,¹³ photovoltaic cells,¹⁴ copying materials,¹⁵ photoreceptors,¹⁶ lithographic printing plates,¹⁷ inks,¹⁸ toner,¹⁹ paints,²⁰ textiles,^{21,22} detecting cancer²³

Safety/Toxicity Oral acute toxicity,²⁴ acute contact dermatitis²⁵

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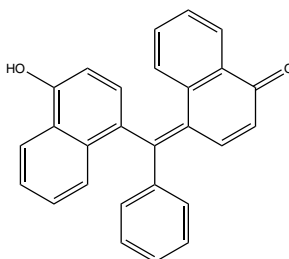
α -NAPHTHOLBENZEIN

Other Names 1(4H)-Naphthalenone, 4-[α -(4-hydroxy-1-naphthyl)benzylidene]-; α -Naphtholbenzein; NSC 9862; *p*-Naphtholbenzein

CA Index Name: 1(4H)-Naphthalenone, 4-[(4-hydroxy-1-naphthalenyl)-phenylmethylene]-

CAS Registry Number 145-50-6

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Benzein

Molecular Formula C₂₇H₁₈O₂

Molecular Weight 374.43

pH Range 0.0-0.8;

8.2-11.0

Color Change at pH Green (0.0) to yellow (0.8)

Yellow (8.2) to green-blue (11.0)

pKa 8.95

Physical Form Red-brown powder

Solubility Insoluble in water; soluble in ethanol, methanol

UV-Visible (λ_{max}) 210 nm

Melting Point 230-235°C

Boiling Point (Calcd.) 578.6 $\pm$ 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods¹⁻³

Applications Semiconducting polymers,⁴ concrete,⁵ correction fluid,⁶ food storage,⁷ determining bacterial growth in packed food,⁸ personal hygiene products,⁹ detecting viable cells,¹⁰ detecting enzymes,¹¹ detecting ammonia odors in patients having bacterial infection¹²

Safety/Toxicity Acute oral toxicity¹³

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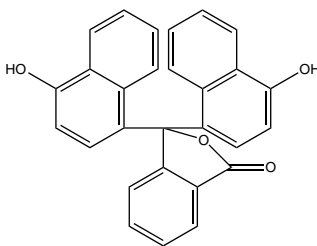
α -NAPHTHOLPHTHALEIN

Other Names 1,1'-Naphthol-4,4'-phthalein; Phthalide, 3,3-bis(4-hydroxy-1-naphthyl)-; α -Naphtholphthalein; 1-Naphtholphthalein; 3,3-Bis(4-hydroxy-1-naphthyl)-1,3-dihydroisobenzofuran-1-one; 3,3-Bis(4-hydroxy-1-naphthyl)phthalide; Di-*p*- α -Naphtholphthalide; Naphtholphthalein blue; *p*- α -Naphtholphthalein

CA Index Name 1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxy-1-naphthalenyl)-

CAS Registry Number 596-01-0

Merck Index Number 6389

Chemical Structure

Chemical/Dye Class Phthalein

Molecular Formula C₂₈H₁₈O₄

Molecular Weight 418.44

pH Range 7.3–8.7

Color Change at pH Colorless (7.3) to greenish-blue (8.7)

pKa 8.0, 8.2, 8.5

Physical Form Colorless powder when pure, usually grayish-red powder

Solubility Practically insoluble in water; soluble in ethanol

UV-Visible (λ_{max}) 648 nm

Melting Point 253–255°C

Boiling Point (Calcd.) 705.6 $\pm$ 60.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Applications Sensors,^{3,4} sol-gel materials,⁵ thermochromic materials,⁶ recording materials,⁷ imaging materials,⁸ authentication system for secure documents,⁹ inks,¹⁰ markers,¹¹ toners,¹² paints,¹³ adhesives,¹⁴ rubber,¹⁵ lubricants,¹⁶ food storage,¹⁷ fruits or vegetable packaging,¹⁸ detecting viable cells,¹⁹ drugs,²⁰ oral hygiene products,²¹ dental materials²²

Safety/Toxicity No data available

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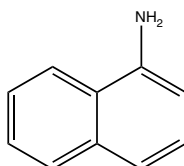
α -NAPHTHYLAMINE

Other Names 1-Naphthylamine; α -Aminonaphthalene; α -Naphthylamine; 1-Aminonaphthalene; 1-Naphthalamine; C.I. 37265; C.I. Azoic Diazo Component 114; Fast Garnet Base B; Naphthalen-1-ylamine; Naphthalidam; Naphthalidine

CA Index Name 1-Naphthalenamine

CAS Registry Number 134-32-7

Merck Index Number 6398

Chemical Structure

Chemical/Dye Class Fluorescent

Molecular Formula $C_{10}H_9N$

Molecular Weight 143.19

pH Range 3.4–4.8

Color Change at pH Nonfluorescence (3.4) to blue fluorescence (4.8)

pKa 3.94

Physical Form Reddish needles

Solubility Slightly soluble in water; freely soluble in ethanol, ether

Melting Point 50°C

Boiling Point 301°C

Synthesis Synthetic methods^{1–12}

Major Applications Color filter,¹³ photoresists,¹⁴ recording media,¹⁵ light-emitting device,¹⁶ optical disk,¹⁷ display device,¹⁸ oil products,¹⁹ construction materials,²⁰ leather,²¹ textile,²² chalk,²³ detecting explosives²⁴

Safety/Toxicity Carcinogenicity,²⁵ chemical toxicity,²⁶ genotoxicity,²⁷ hepatotoxicity,²⁸ mutagenicity,²⁹ phytotoxicity³⁰

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β -NAPHTHYLAMINE

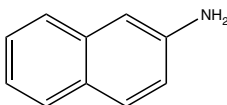
Other Names 2-Naphthylamine; β -Aminonaphthalene; β -Naphthylamine; 2-Aminonaphthalene; C.I. 37270; Fast Scarlet Base B; Naphthalen-2-ylamine; *o*-Aminonaphthalene

CA Index Name 2-Naphthalenamine

CAS Registry Number 91-59-8

Merck Index Number 6399

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula C₁₀H₉N

Molecular Weight 143.19

pH Range 2.8–4.4

Color Change at pH Nonfluorescence (2.8) to violet fluorescence (4.4)

pKa 4.20

Physical Form White to reddish crystals

Solubility Soluble in hot water, ethanol, ether

Melting Point 111–113°C

Boiling Point 306°C

Synthesis Synthetic methods^{1–4}

Major Applications Microelectronics,⁵ power transmission fluid,⁶ insulators for electronic devices,⁷ photoresists,⁸ display device,⁹ imaging process,¹⁰ semiconductors,¹¹ diesel fuel additives,¹² battery,¹³ adhesive,¹⁴ paints,¹⁵ inks,¹⁶ chalk,¹⁷ leather,¹⁸ textiles,¹⁸ dye synthesis,¹⁹ soil products²⁰

Safety/Toxicity Carcinogenicity,^{21,22} cytotoxicity,²³ genotoxicity,²³ mutagenicity,²⁴ tumorigenicity²⁵

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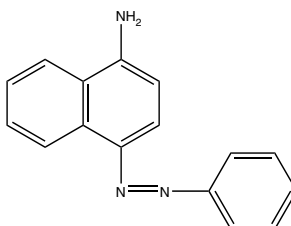
α -NAPHTHYL RED

Other Names 1-Naphthylamine, 4-phenylazo-; C.I. Solvent Yellow 4; α -Naphthyl red; 4-(Phenylazo)- α -naphthylamine; 4-(Phenylazo)-1-naphthylamine; 4-Benzeneazo-1-naphthylamine; C.I. 11350; NSC 13974; Nubian Yellow TB

CA Index Name 1-Naphthalenamine, 4-(phenylazo)-

CAS Registry Number 131-22-6

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Azo

Molecular Formula $C_{16}H_{13}N_3$

Molecular Weight 247.29

pH Range 3.7–5.0

Color Change at pH Red (3.7) to yellow (5.0)

pKa 2.70

Physical Form Dark red crystals

Solubility Virtually insoluble in water; slightly soluble in ethanol; soluble in acetone, benzene, ethyl acetate, toluene, xylene

UV-Visible ($\lambda_{\max}$) 439 nm

Melting Point 124°C

Boiling Point (Calcd.) $451.4 \pm 20.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods^{1–4}

Major Applications Display device,⁵ semiconductor,⁶ sensors,⁷ photosensitive materials,⁸ recording materials,⁹ imaging materials,¹⁰ inks,¹¹ engraving coatings,¹² lubricants,¹³ hair dyes,¹⁴ food storage,^{15,16} dental materials^{17,18}

Safety/Toxicity oral toxicity,¹⁹ mutagenicity²⁰

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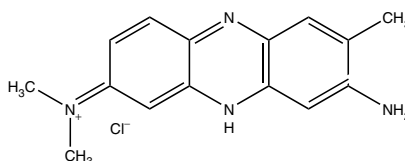
NEUTRAL RED

Other Names C.I. Basic Red 5, monohydrochloride; Toluylene red; 3-Amino-7-dimethylamino-2-methylphenazine hydrochloride; C.I. 50040; C.I. Basic Red 5; Neutral Red; Neutral Red W; Nuclear Fast Red (basic dye)

CA Index Name 2,8-Phenazinediamine, N8,N8,3-trimethyl-, monohydrochloride

CAS Registry Number 553-24-2

Merck Index Number 6488

Chemical Structure

Chemical/Dye Class Miscellaneous, Azine

Molecular Formula C₁₅H₁₆N₄.HCl

Molecular Weight 288.78

pH Range 6.8–8.0

Color Change at pH Red (6.8) to yellow (8.0)

pKa 6.7, 7.4

Physical Form Dark green or brownish-black powder

Solubility Soluble in water, ethanol; practically insoluble in xylene

UV-Visible (λ_{max}) 540 nm, 533 nm, 544 nm, 529 nm, 454 nm

Melting Point 290°C (decompose)

Synthesis Synthetic methods^{1–5}

Major Applications Fuel cell power generation system,⁶ liquid crystal displays,⁷ solar cells,⁸ sensors,⁹ thermochromic materials,¹⁰ coloring wood,¹¹ detergents,¹² assessment of tobacco smoke,¹³ cosmetics,¹⁴ detect bacterial infections,¹⁵ multidrug resistance inhibitors,¹⁶ treatment of burns,¹⁷ endodontic,¹⁸ diabetes,¹⁹ obesity,¹⁹ cancer,²⁰ age-related macular degeneration,²¹ viral diseases²²

Safety/Toxicity Acute toxicity,²³ combustion toxicity,²⁴ cytotoxicity,²⁵ genotoxicity,²⁶ mutagenicity,²⁷ nephrotoxicity,²⁸ phototoxicity,²⁹ soil toxicity³⁰

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NILE BLUE

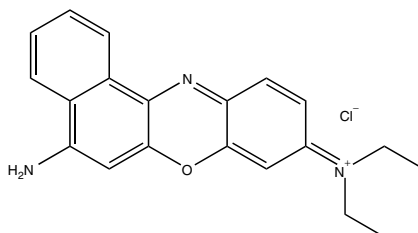
Other Names C.I. Basic Blue 12; Nile Blue; C.I. 51180; Cresol Fast Violet; Cresyl Fast Violet; Nile Blue AX; Nile Blue BX; Nile blue base; Nile blue chloride

CA Index Name Benzo[a]phenoxazin-7-ium, 5-amino-9-(diethylamino)-, chloride

CAS Registry Number 2381-85-3

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Miscellaneous, Oxazine

Molecular Formula C₂₀H₂₀N₃OCl

Molecular Weight 353.85

pH Range 9.4–11.0

Color Change at pH Blue (9.4) to purple-red (11.0)

pKa 9.7

Physical Form Green powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 638 nm

Melting Point >250°C

Synthesis Synthetic methods^{1–3}

Major Applications CMOS technology,⁴ waveguides,⁵ electroluminescent device,⁶ inks,⁷ plastics,⁸ biofuel cells,⁹ detect bacterial growth,¹⁰ lipids,¹¹ DNA,¹² diagnosis of diseases related to amyloid accumulation,¹³ fluorescent probes,¹⁴ therapy of viral diseases,¹⁵ photodynamic therapy¹⁶

Safety/Toxicity Carcinogenicity,¹⁷ cytotoxicity,¹⁸ mutagenicity,¹⁹ teratogenicity²⁰

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NITRAMINE

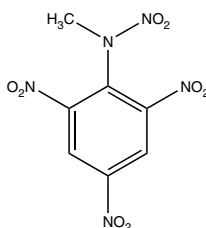
Other Names Aniline, *N*-methyl-*N*,2,4,6-tetranitro-; 2,4,6-*N*-Tetranitro-*N*-methylaniline; 2,4,6-Tetryl; 2,4,6-Trinitro-*N*-methyl-*N*-nitroaniline; 2,4,6-Trinitrophenyl-*N*-methylnitramine; 2,4,6-Trinitrophenylmethylnitroamine; CE; *N*-Methyl-*N*,2,4,6-tetranitroaniline; *N*-Methyl-*N*-picrylnitramine; *N*-Picryl-*N*-methylnitramine; NSC 2166; Nitramine; Nitramine (indicator); Picrylmethylnitramine; Picrylnitromethylamine; Tetralit; Tetralite; Tetril; Tetryl

CA Index Name Benzenamine, *N*-methyl-*N*,2,4,6-tetranitro-

CAS Registry Number 479-45-8

Merck Index Number 6573

Chemical Structure



Chemical/Dye Class Nitro

Molecular Formula $C_7H_5N_5O_8$

Molecular Weight 287.14

pH Range 10.8–13.0

Color Change at pH Colorless (10.8) to red-brown (13.0)

pKa 12.66

Physical Form Yellow crystals

Solubility Insoluble in water; soluble in ethanol, ether, benzene, acetic acid

Melting Point 130–132°C

Boiling Point (Calcd.) $503.7 \pm 50.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods^{1–11}

Major Applications Explosives,^{2–3,9–17} paints,¹⁸ food storage¹⁹

Safety/Toxicity Cytotoxicity,²⁰ marine toxicity,²¹ mutagenicity,^{22,23} genotoxicity²⁴

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NITRAZINE YELLOW

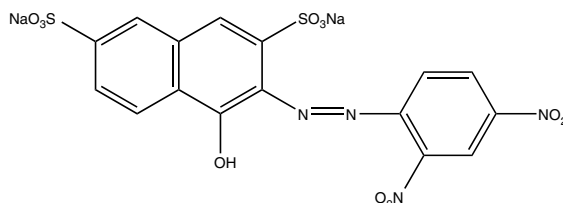
Other Names Nitrazine yellow; C.I. 14890; Delta Paper; Nitrazol Yellow

CA Index Name 2,7-Naphthalenedisulfonic acid, 3-[(2,4-dinitrophenyl)azo]-4-hydroxy-, disodium salt

CAS Registry Number 5423-07-4

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula $C_{16}H_8N_4O_{11}S_2Na_2$

Molecular Weight 542.37

pH Range 6.0–7.2

Color Change at pH Bright yellow (6.0) to bright blue (7.2)

Physical Form Red-brown powder

Solubility Soluble in water, acetic acid ethanol

UV-Visible (λ_{max}) 586 nm

Melting Point >250°C

Synthesis Synthetic methods^{1,2}

Major Applications Sensors,^{3–5} display devices,⁶ sol-gel matrix,⁷ electrorheological materials,⁸ diesel fuels/kerosines,⁹ detergent,¹⁰ fabric softener,¹¹ food storage,¹² method for identifying fresh & stale rice,¹³ in dialysis solution,¹⁴ screening of NAD-binding,¹⁵ monitoring secreted body fluids,¹⁶ locating lymph node,¹⁷ diagnostic pads,¹⁸ vaginal infection test method,¹⁹ assay for esterolytic enzyme activity,²⁰ detecting pathogenic bacteria,²¹ diagnosis of bacterial vaginosis,²² detecting dysfunctional pregnancy,²³ drugs screening^{24,25}

Safety/Toxicity No data available

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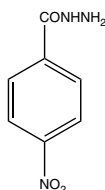
***p*-NITROBENZHYDRAZIDE**

Other Names Benzoic acid, *p*-nitro-, hydrazide; (*p*-Nitrobenzoyl)hydrazine; 4-Nitrobenzenecarboxylic acid hydrazide; 4-Nitrobenzhydrazide; 4-Nitrobenzohydrazide; 4-Nitrobenzoic acid hydrazide; 4-Nitrobenzoic hydrazide; 4-Nitrobenzoyl hydrazide; 4-Nitrobenzoylhydrazine; INHd 18; NSC 9804; *p*-Nitrobenzhydrazide; *p*-Nitrobenzohydrazide; *p*-Nitrobenzoic acid hydrazide; *p*-Nitrobenzoic hydrazide; *p*-Nitrobenzoyl hydrazide

CA Index Name Benzoic acid, 4-nitro-, hydrazide

CAS Registry Number 636-97-5

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Miscellaneous, Nitro, Hydrazide

Molecular Formula C₇H₇N₃O₃

Molecular Weight 181.15

pH Range 8.2–9.5

Color Change at pH Colorless (8.2) to yellow (9.5)

pKa 2.77, 11.17

Physical Form Yellow crystals

Solubility Insoluble in water; soluble in ethanol, methanol

UV-Visible (λ_{max}) 267 nm

Melting Point 218°C (decompose)

Synthesis Synthetic methods^{1–9}

Major Applications corrosion inhibitor,^{10,11} disinfectant,¹ cosmetics,² paints³ toothpaste,⁴ mouthwash,⁴ antifungal agent,¹² inhibit fibrosis,¹³ antituberculosis agent¹⁴

Safety/Toxicity Toxicity,¹⁵ teratogenicity,¹⁶ acute oral toxicity¹⁷

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***p*-NITROBENZYL CYANIDE**

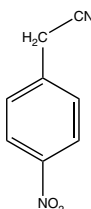
Other Names Acetonitrile, (*p*-nitrophenyl)-; (*p*-Nitrophenyl)acetonitrile; 4-Nitrobenzeneacetonitrile; 4-Nitrobenzyl cyanide; 4-Nitrophenylacetonitrile; NSC 5396; *p*-Nitro- α -tolunitrile; *p*-Nitrobenzeneacetonitrile; *p*-Nitrobenzyl cyanide

CA Index Name Benzeneacetonitrile, 4-nitro-

CAS Registry Number 555-21-5

Merck Index Number 6591

Chemical Structure



Chemical/Dye Class Miscellaneous, Nitro

Molecular Formula $C_8H_6N_2O_2$

Molecular Weight 162.15

pH Range 11.4–12.9

Color Change at pH Yellow (11.4) to Orange-red (12.9)

Physical Form Yellow powder

Solubility Insoluble in water, soluble in ethanol, ether

Melting Point 117°C

Boiling Point (Calcd.) $336.3 \pm 17.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods^{1–18}

Major Applications Recording materials,^{19,20} photography,^{21,22} forge-proof security paper,²³

Safety/Toxicity toxicology,²⁴ acute toxicity,²⁵ oral toxicity²⁶

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4-NITROCATECHOL

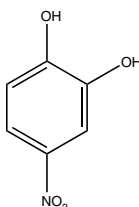
Other Names Pyrocatechol, 4-nitro-; 1,2-Dihydroxy-4-nitrobenzene; 3,4-Dihydroxy-1-nitrobenzene; 3,4-Dihydroxynitrobenzene; 4-Nitro-1,2-benzenediol; 4-Nitro-1,2-dihydroxybenzene; 4-Nitrobenzocatechin; 4-Nitrocatechol; 4-Nitropyrocatechol; NSC 80651; *p*-Nitrocatechol

CA Index Name 1,2-Benzenediol, 4-nitro-

CAS Registry Number 3316-09-4

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Nitro

Molecular Formula $C_6H_5NO_4$

Molecular Weight 155.11

pH Range 3.9–6.3

Color Change at pH Straw (3.9) to lemon yellow (6.3)

pKa 6.84

Physical Form Light yellow crystals

Solubility Very slightly soluble in water; soluble in ethanol

UV-Visible (λ_{max}) 385 nm, 510 nm

Melting Point 174–176°C

Boiling Point (Calcd.) $358.2 \pm 32.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods^{1–12}

Major Applications Semiconductors,¹³ magnetic recording materials,¹⁴ nonlinear optical materials,¹⁵ photography,¹⁶ determination of lysosomal enzyme disorders,¹⁷ antimicrobial agent,¹⁸ anti-cancer agent¹⁹

Safety/Toxicity Chemistry-toxicity relationship,²⁰ ecotoxicity,²¹ toxicity,²² cytotoxicity,²³ phytotoxicity²⁴

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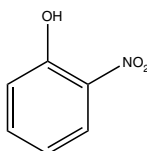
o-NITROPHENOL

Other Names Phenol, *o*-nitro-; 2-Hydroxynitrobenzene; 2-Nitrophenol; NSC 1552; *o*-Hydroxynitrobenzene; *o*-Nitrophenol

CA Index Name Phenol, 2-nitro-

CAS Registry Number 88-75-5

Merck Index Number 6620

Chemical Structure

Chemical/Dye Class Nitro

Molecular Formula C₆H₅NO₃

Molecular Weight 139.11

pH Range 5.0–7.0

Color Change at pH Colorless (5.0) to yellow (7.0)

pKa 7.14, 7.22

Physical Form Light yellow crystals

Solubility Sparingly soluble in water; soluble in ethanol, ether, benzene

Melting Point 44–45°C

Boiling Point 214–216°C

Synthesis Synthetic methods^{1–12}

Major Applications High voltage capacitors,^{13,14} inks,¹⁵ energetic materials,¹⁶ corrosion inhibitors,^{17,18} fertilizer,¹⁹ food storage,²⁰ enzyme assays,²¹ detecting microorganisms,²² immunotherapy,²³ drugs²⁴

Safety/Toxicity Chemical toxicity,^{25,26} ecotoxicity,²⁷ acute toxicity,²⁸ toxicology,²⁹ mutagenicity,³⁰ immunotoxicology,³¹ genotoxicity,³² hepatotoxicity,³³ cytotoxicity,³³ phytotoxicity³⁴

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***m*-NITROPHENOL**

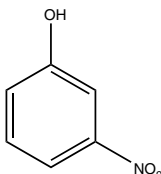
Other Names Phenol, *m*-nitro-; 1-Hydroxy-3-nitrobenzene; 3-Hydroxynitrobenzene; 3-Nitrophenol; NSC 1551; *m*-Hydroxynitrobenzene; *m*-Nitrophenol

CA Index Name Phenol, 3-nitro-

CAS Registry Number 554-84-7

Merck Index Number 6619

Chemical Structure



Chemical/Dye Class Nitro

Molecular Formula C₆H₅NO₃

Molecular Weight 139.11

pH Range 6.8–8.6

Color Change at pH Colorless (6.8) to yellow (8.6)

pKa 8.34, 8.30, 8.33

Physical Form Yellow to orange-brown crystals

Solubility Sparingly soluble in water; soluble in ethanol

UV-Visible (λ_{max}) 570 nm

Melting Point 97–98°C

Boiling Point 277°C

Synthesis Synthetic methods^{1–11}

Major Applications Display device,¹² semiconductor device,¹³ sensors,¹⁴ high voltage capacitors,¹⁵ energetic materials,¹⁶ electrolyte batteries,¹⁷ inks,¹⁸ correction fluid,¹⁹ detergent,²⁰ leak detection method,²¹ lubricants,²² insecticide,²³ food storage,²⁴ inhibition of amyloidoses,²⁵ detect bacterial infection,²⁶ drugs,²⁷ material for evaluating dental caries activity²⁸

Safety/Toxicity Chemical toxicity,^{29,30} ecotoxicity,³¹ acute toxicity,³² toxicology,³³ mutagenicity,³⁴ immunotoxicology,³⁵ genotoxicity,³⁶ hepatotoxicity,³⁷ cytotoxicity,³⁷ phytotoxicity³⁸

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37. Shoji, R.; Sakoda, A.; Sakai, Y.; Utsumi, H.; Suzuki, M. A new assay for evaluating hepatotoxicity and cytotoxicity using LDL-uptake activity of liver cells. *J. Health Sci.* **2000**, *46*, 493–502.
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p-NITROPHENOL

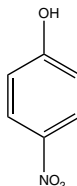
OtherNames Phenol,*p*-nitro-; 1-Hydroxy-4-nitrobenzene; 4-Hydroxy-1-nitrobenzene; 4-Hydroxynitrobenzene; 4-Nitrophenol; NSC 1317; Niphen; *p*-Hydroxynitrobenzene; *p*-Nitrophenol

CA Index Name Phenol, 4-nitro-

CAS Registry Number 100-02-7

Merck Index Number 6621

Chemical Structure



Chemical/Dye Class Nitro

Molecular Formula C₆H₅NO₃

Molecular Weight 139.11

pH Range 5.6–7.6

Color Change at pH Colorless (5.6) to yellow (7.6)

pKa 7.15

Physical Form Yellow crystals

Solubility Sparingly soluble in water; soluble in ethanol, ether, chloroform

UV-Visible (λ_{max}) 320 nm, 405 nm

Melting Point 113–114°C

Boiling Point 279°C

Synthesis Synthetic methods^{1–15}

Major Applications Display device,¹⁶ solar cells,¹⁷ nanoparticles,¹⁸ electrolytic capacitors,^{19,20} lithographic printing plate,²¹ leak detection method,²² falsification-proof security paper,²³ correction fluid,²⁴ detergent,²⁵ fertilizer,²⁶ identifying fresh and stale rice,²⁷ diapers,²⁸ detecting lactic acid bacteria,²⁹ drug delivery,³⁰ evaluating dental caries activity³¹

Safety/Toxicity Aquatic toxicity,³² chemical toxicity,³³ cytotoxicity,³⁴ ecotoxicity,³⁵ genotoxicity,³⁶ hepatotoxicity,³⁷ immunotoxicity,³⁷ mutagenicity,³⁸ neurotoxicity³⁹

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O

ORANGE II

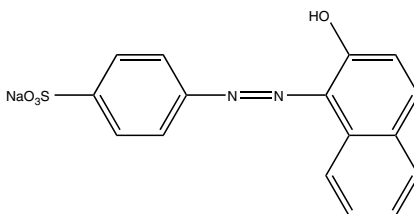
Other Names Acid Orange; Acid Orange A; C.I. Acid Orange 7, monosodium salt; Benzenesulfonic acid, *p*-(2-hydroxy-1-naphthylazo)-, sodium salt; β -Naphthol Orange; β -Naphthyl orange; 11550 Orange; 2-Naphthol Orange II; AO 7; Acid Leather Orange PRW; Acid Leather Orange extra; Acid Orange 7; Acid Orange II; Acilan Orange II; Airedale Orange II; Amacid Orange Y; Amacid Orange Y Conc; Atul Acid Orange II; Basacid Orange 280; Basacid Orange 282; Betanaphthol orange; Brasilan Orange A; Bucacid Orange A; C Ext. Orange 8; C.I. 15510; C.I. Acid Orange 7; Calcocid Orange Y; Certiquel Orange II; Colacid Orange; Curol Orange; D and C Orange No. 4; D&C Orange #4; D&C Orange No. 4; Diacid Orange II; Duasyn Acid Orange P; Egacid Orange II; Erio Orange II; Everacid Orange II; Fenazo Orange; Hidacid Orange II; Hispacid Orange AF; Japan Orange 205; Japan Orange No. 205; Java Orange II; Keyacid Orange II; Kiton Orange II; Kromon Lake Orange Toner; Lake Orange A; Lake Orange II YS; Leather Orange Extra; Lurazol Orange E; Lurazol Orange EBR; Lutetia Orange 3JR; Mandarin G; Naphthalene Lake Orange G; Naphthalene Orange G; Naphthol Orange; Naphtocard Orange II; Neklacid Orange II; No. 177 Orange Lake; Nubilon Orange R; Orange 2; Orange 2 sodium salt; Orange Extra N; Orange Extra P; Orange II; Orange II Special For Lacquer; Orange II for Lakes; Orange IIC; Orange IIP; Orange IIS; Orange IISM; Orange No. 205; Orange Toner GRT; Orange Y; Orange YA; Orange YZ; Peer-acid Orange II; Persian Orange; Persian Orange Lake; Persian Orange X; Pure Orange II S; Rifa Acid Orange II; Rybacel Orange A; Sanyo Gum Orange A; Sodium 4-(2-hydroxy-1-naphthylazo)benzenesulfonate; Solar Orange; Special Orange GR; Special Orange H; Symuler Orange Lake 43; Symulon Acid Orange II; Takaoka Acid Orange II; Tangarine Lake X 917; Tertracid Orange II; Tropaeolin OOO; Tropaeolin OOO 2; Tropeolin OOO; Vondacid Orange II; Wool Orange A; *p*-(2-Hydroxy-1-naphthylazo)benzenesulfonic acid sodium salt

CA Index Name Benzenesulfonic acid, 4-[(2-hydroxy-1-naphthalenyl)azo]-, monosodium salt

CAS Registry Number 633-96-5

Merck Index Number 6858

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula $C_{16}H_{11}N_2O_4SNa$

Molecular Weight 350.33

pH Range 7.4–8.6;

10.2–11.8

Color Change at pH Amber (7.4) to orange (8.6)

Orange (10.2) to red (11.8)

pKa 8.26, 11.4

Physical Form Orange-brown powder

Solubility Very soluble in water; very slightly soluble in ethanol

UV-Visible (λ_{max}) 483 nm

Melting Point >300°C

Synthesis Synthetic methods^{1–6}

Major Applications Organic light emitting diodes (OLEDs),⁷ nanoparticles,⁸ inks,⁹ wood preservatives,¹⁰ textiles,¹¹ hair dyes,^{12,13} cosmetics,^{14,15} wound dressing materials,¹⁶ biofuel cells¹⁷

Safety/Toxicity Acute toxicity,¹⁸ carcinogenicity,¹⁹ genotoxicity,²⁰ toxicity to fish,²¹ mutagenicity^{22,23}

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ORANGE III

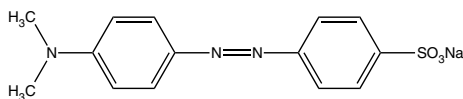
Other Names Benzenesulfonic acid, *p*-[[*p*-(dimethylamino)phenyl]azo]-, sodium salt; Orange III; 4-Dimethylaminoazobenzene-4'-sulfonic acid sodium salt; C.I. 13025; C.I. Acid Orange 52; Diazoben; Eniamethyl Orange; Gold orange; Helianthine; Helianthine B; KCA Methyl Orange; Methyl Orange B; Methyl orange; Orange 3; Sodium 4'-(dimethylamino)azobenzene-4-sulfonate; Sodium 4-(dimethylamino)azobenzene-4'-sulfonate; Sodium 4-[4-(dimethylamino)-phenylazo]-benzenesulfonate; Sodium *p*-[*p*-(dimethylamino)-phenylazo]-benzenesulfonate; Sodium *p*-dimethylaminoazobenzenesulfonate; Tropaeolin D

CA Index Name Benzenesulfonic acid, 4-[[4-(dimethylamino)phenyl]azo]-, sodium salt

CAS Registry Number 547-58-0

Merck Index Number 6105

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula C₁₄H₁₄N₃O₃SNa

Molecular Weight 327.34

pH Range 3.0–4.4

Color Change at pH Red (3.0) to yellow (4.4)

pKa 3.76, 3.40

Physical Form Orange powder

Solubility Slightly soluble in water, more soluble in hot water; practically insoluble in ethanol

UV-Visible (λ_{max}) 507 nm, 522 nm, 464 nm

Melting Point >300°C

Synthesis Synthetic methods^{1–9}

Major Applications Liquid crystals,¹⁰ thin films,¹¹ sensors,¹² sol-gel matrix,¹³ waveguides,¹⁴ host-guest chemistry,¹⁵ display device,¹⁶ corrosion inhibitor,¹⁷ glass coatings,¹⁸ paints,¹⁹ wound dressing materials,²⁰ pharmaceuticals,²¹ dental materials,²² measuring nucleic acid²³

Safety/Toxicity Carcinogenicity,²⁴ genotoxicity,²⁵ mutagenicity²⁶

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ORANGE IV

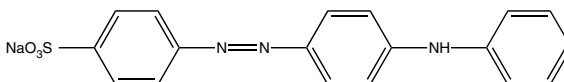
Other Names Benzenesulfonic acid, *p*-(*p*-anilinophenylazo)-, sodium salt; C.I. Acid Orange 5; C.I. Acid Orange 5, monosodium salt; Acid Orange 5; Acid Orange IV; Acid Yellow D; Aniline Yellow; C.I. 13080; Diphenylamine Orange; Hispacid Orange IV; Orange GS; Orange IV; Orange N; Solar Orange IV; Tertracid Orange IV; Tropaeolin OO; Tropeolin OO

CA Index Name Benzenesulfonic acid, 4-[[4-(phenylamino)phenyl]azo]-, monosodium salt

CAS Registry Number 554-73-4

Merck Index Number 9776

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula C₁₈H₁₄N₃O₃SNa

Molecular Weight 375.38

pH Range 1.4–2.6

Color Change at pH Red (1.4) to yellow (2.6)

pKa 2.0

Physical Form Orange-yellow powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 527 nm, 443 nm

Melting Point >300°C

Synthesis Synthetic methods^{1–4}

Major Applications Sensors,⁵ lithographic plates,⁶ optical recording media,⁷ photoreceptor,⁸ inks,⁹ indication system for product exceeding threshold temperature,¹⁰ lubricants,¹¹ textiles,¹² food storage,¹³ determination of amiodarone,¹⁴ astemizole,¹⁵ bromhexine,¹⁶ clomipramine,¹⁷ deuterforin,¹⁸ domperidone,¹⁹ fluoroquinolone,²⁰ roxithromycin,²¹ terfenadine,²² thiabendazole,²³ antihistamines²⁴

Safety/Toxicity Biodegradation and toxicity²⁵

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OREGON GREEN 488 CARBOXYLIC ACID

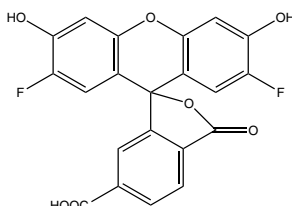
Other Names Oregon Green 488 carboxylic acid

CA Index Name Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid, 2',7'-difluoro-3',6'-dihydroxy-3-oxo-

CAS Registry Number 195136-52-8

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula C₂₁H₁₀F₂O₇

Molecular Weight 412.30

pH Range 4.2–5.7

Color Change at pH Weak green fluorescence (4.2) to strong green fluorescence (5.7)

pKa 4.7

Physical Form Solid

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide

UV-Visible (λ_{max}) 478 nm, 492 nm

Melting Point >250°C

Boiling Point (Calcd.) 693.9 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–3}

Major Applications Sensors,⁴ methods of determining human blood-relationship,⁵ method for purifying actin in plant cells,⁶ phagosomal pH determination⁷

Safety/Toxicity No data available

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OREGON GREEN 514 CARBOXYLIC ACID

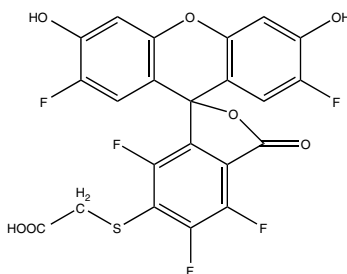
Other Names Oregon Green 514 carboxylic acid 6-isomer

CA Index Name Acetic acid, [(2',4,5,7,7'-pentafluoro-3',6'-dihydroxy-3-oxospiro-[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl)thio]-

CAS Registry Number 198139-49-0

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula C₂₂H₉F₅O₇S

Molecular Weight 512.36

pH Range 4.2–5.7

Color Change at pH Weak green fluorescence (4.2) to strong green fluorescence (5.7)

pKa 4.7

Physical Form Solid

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide

UV-Visible (λ_{max}) 489 nm, 506 nm

Melting Point >250°C

Boiling Point (calcd.) 703.2 ± 60.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–3}

Major Applications Method for measuring stress biomarkers in body fluids,⁴ method for diagnostic & therapeutic transport,⁵ monitoring protein conformation,⁶ detecting bacteria,⁷ delivering nucleic acids & proteins across skin,⁸ method for determining size of polynucleotides,⁹ probing the diffusion in ultrathin films,¹⁰ genotyping of nucleic acid polymorphisms,¹¹ molecular clasps,¹² measuring protein–protein & protein–nucleic acid interactions,¹³ analysis of the protein distribution,¹⁴ detecting gene expression,¹⁵ as geothermal tracers,¹⁶ determination of biomolecules,¹⁷ pH sensors¹⁸

Safety/Toxicity No data available

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OREGON GREEN 488 CARBOXYLIC ACID DIACETATE

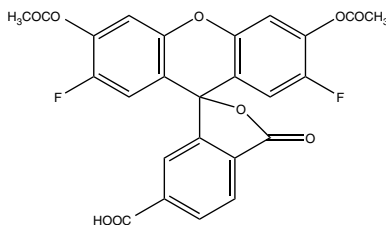
Other Names Oregon Green 488 carboxylic acid diacetate

CA Index Name Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid, 3',6'-bis(acetyloxy)-2',7'-difluoro-3-oxo-

CAS Registry Number 195136-74-4

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Xanthene

Molecular Formula C₂₅H₁₄F₂O₉

Molecular Weight 496.37

pH Range 4.2–5.7

Color Change at pH Weak green fluorescence (4.2) to strong green fluorescence (5.7)

pKa 4.65

Physical Form Solid

Solubility Insoluble in water; soluble in *N,N*-dimethyl formamide, dimethyl sulfoxide

UV-Visible (λ_{max}) <300 nm

Melting Point >250°C

Boiling Point (Calcd.) 691.5 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Electrical lysis of cells,³ detecting anion transport mechanism at the tonoplast,⁴ as tracers and for preparing conjugates of organic & inorganic substances¹

Safety/Toxicity No data available

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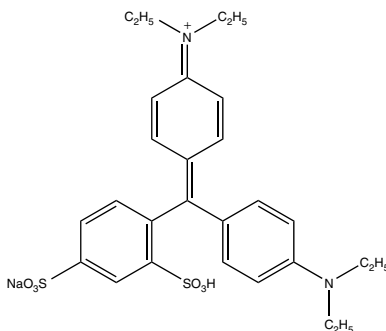
PATENT BLUE V

Other Names C.I. Acid Blue 1, sodium salt; Ethanaminium, *N*-[4-[[4- (diethylamino)phenyl](2, 4-disulphophenyl)methylene]-2,5-cyclohexadien-1-ylidene]-*N*-ethyl-, hydroxide, inner salt, sodium salt; Xylene Blue VS; [4-[α -[*p*-(Diethylamino)phenyl]-2,4-isulphobenzylidene]-2,5-cyclohexadien-1-ylidene]-diethylammonium hydroxide, inner salt, sodium salt; 1085 Blue; Acid Blue 1; Acid Blue V; Acid Bright Azure Z; Acid Brilliant Blue Z; Acid Brilliant Sky Blue Z; Acid Leather Blue V; Acid Turquoise Blue V; Aizen Brilliant Acid Pure Blue VH; Alphazurine 2G; Amacid Blue V; Bleu Patente V; Blue URS; Blue VRS; Brilliant Acid Blue A Export; Brilliant Acid Blue V Extra; Brilliant Acid Blue VS; Brilliant Blue GS; Bucacid Patent Blue VF; C.I. 42045; C.I. Acid Blue 1; C.I. Food Blue 3; Carmine Blue VF; Disulfine blue VN; Disulphine Blue VN; Disulphine Blue VN 150; Disulphine VN; Duasyn Acid Blue V 02; Edicol Supra Blue VR; Erioglaucine supra; Fenazo Blue XF; Hexacol Blue VRS; Hidacid Blue V; Kiton Pure Blue V; Kiton Pure Blue V.FQ; Leather Blue G; Merantine Blue VF; Orient Water Blue 106; Patent Blue; Patent Blue V; Patent Blue VF; Patent Blue VF Special; Patent Blue VF-CF; Patent Pure Blue VX; Patent blue VS; Patent blue violet; Pontacyl Brilliant Blue V; Sodium Blue VRS; Sodium Patent Blue V; Sulfan blue; Sulphan Blue; Sumitomo Patent Pure Blue VX; Tertracid Carmine Blue V

CA Index Name Ethanaminium, *N*-[4-[[4-(diethylamino)phenyl](2,4- disulphophenyl)methylene]-2,5-cyclohexadien-1-ylidene]-*N*-ethyl-, inner salt, sodium salt

CAS Registry Number 129-17-9

Merck Index Number 8987

Chemical Structure

Chemical/Dye Class Triphenylmethane

Molecular Formula $C_{27}H_{31}N_2O_6S_2Na$

Molecular Weight 566.68

pH Range 0.8–3.0

Color Change at pH Yellow-orange (0.8) to deep blue (3.0)

Physical Form Dark blue powder

Solubility Soluble in water; partly soluble in ethanol; insoluble in xylene

UV-Visible (λ_{max}) 635 nm, 410 nm

Melting Point >250°C

Synthesis Synthetic methods^{1–3}

Major Applications Liquid crystal displays,⁴ color filters,^{5,6} electrorheological materials,⁷ photographic materials,⁸ optical filters,⁹ inks,¹⁰ highlighters,¹¹ dyeing paper,¹² wood dyeing,¹³ textiles,¹⁴ detergents,¹⁵ hair dyes,¹⁶ cosmetics,¹⁷ lymph node identification,¹⁸ antiparasitic agent,¹⁹ nanocomposite particles for biomedical applications²⁰

Safety/Toxicity Acute toxicity,²¹ genotoxicity,²² mutagenicity,^{23,24} allergic reaction,²⁵ adverse reaction²⁶

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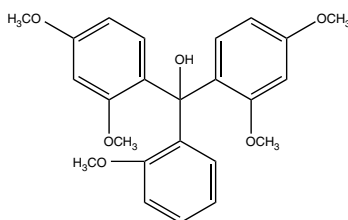
PENTAMETHOXY RED

Other Names Methanol, *bis*(2,4-dimethoxyphenyl)(*o*-methoxyphenyl)-; 2,2',2'',4,4'-Pentamethoxytriphenylcarbinol; Pentamethoxy Red

CA Index Name Benzenemethanol, α -(2,4-dimethoxyphenyl)-2,4-dimethoxy- α -(2-methoxyphenyl)-

CAS Registry Number 1755-51-7

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Triphenylmethane

Molecular Formula C₂₄H₂₆O₆

Molecular Weight 410.46

pH Range 1.2–3.2

Color Change at pH Reddish-violet (1.2) to colorless (3.2)

pKa 1.86

Physical Form White crystals

Solubility Insoluble in water; soluble in ethanol

Melting Point 146–148°C

Boiling Point (Calcd.) 600.3 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–5}

Major Applications Image producing materials,^{6–9} recording materials,^{10–12} resist composition,¹³ xerographic copier materials,¹⁴ inks,¹⁵ cleaners,¹⁶ cosmetics,¹⁶ dental adhesives,¹⁷

Safety/Toxicity No data available

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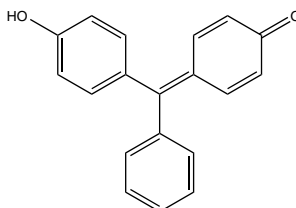
PHENOLBENZEIN

Other Names 2,5-Cyclohexadien-1-one, 4-(*p*-hydroxy- α -phenylbenzylidene)-; Benzaurin; NSC 55861; Phenolbenzein; Rosolic acid

CA Index Name 2,5-Cyclohexadien-1-one, 4-[(4-hydroxyphenyl)phenylmethylene]-

CAS Registry Number 569-60-8

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Benzein

Molecular Formula C₁₉H₁₄O₂

Molecular Weight 274.31

pH Range 6.0–7.6

Color Change at pH Yellow (6.0) to red (7.6)

pKa 9.28

Physical Form Orange-red crystals

Solubility Insoluble in water; soluble in ethanol

Melting Point >250°C

Boiling Point (Calcd.) 497.0 ± 45.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–5}

Major Applications Indicator⁶

Safety/Toxicity No data available

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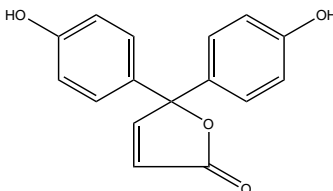
PHENOLMALEIN

Other Names 2(5H)-Furanone, 5,5-bis(*p*-hydroxyphenyl)-; Crotonic acid, 4- hydroxy-4,4-bis(*p*-hydroxyphenyl)-, γ -lactone; Phenolmalein

CA Index Name 2(5H)-Furanone, 5,5-bis(4-hydroxyphenyl)-

CAS Registry Number 1224-25-5

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Miscellaneous

Molecular Formula C₁₆H₁₂O₄

Molecular Weight 268.26

pH Range 5.5–7.2

Color Change at pH Yellow (5.5) to red (7.2)

pKa 6.04

Physical Form Yellow crystals

Solubility Insoluble in water, soluble in ethanol, acetone

Melting Point 301°C

Boiling Point (Calcd.) 533.9 $\pm$ 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Bactericidal activity³

Safety/Toxicity No data available

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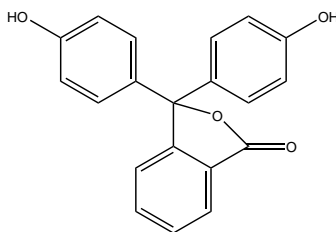
PHENOLPHTHALEIN

Other Names Phenolphthalein; 3,3-Bis(4-hydroxyphenyl)-1(3H)-isobenzofuranone; 3,3-Bis(4-hydroxyphenyl)phthalide; 3,3-Bis(*p*-hydroxyphenyl)phthalide; Euchessina; Koprol; Laxogen; Lilo; NSC 10464; NSC 215214; Phthalimetten; Phthalin; Purga; Purgen; Purgophen; Spulmakolax; Trilax

CA Index Name 1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxyphenyl)-

CAS Registry Number 77-09-8

Merck Index Number 7243

Chemical Structure

Chemical/Dye Class Phthalein

Molecular Formula C₂₀H₁₄O₄

Molecular Weight 318.32

pH Range 8.0–10.0

Color Change at pH Colorless (8.0) to pink (10.0)

pKa 9.10, 9.40, 9.53, 9.70

Physical Form White powder

Solubility Almost insoluble in water; soluble in alcohol, ether

UV-Visible (λ_{max}) 552 nm, 553 nm, 374 nm, 205 nm, 229 nm, 276 nm

Melting Point 258–262°C

Boiling Point (Calcd.) 557.8 ± 50.0°C; Pressure: 760 Torr

Synthesis Synthetic methods^{1–16}

Major Applications Display device,¹⁷ sensors,¹⁸ semiconductors,¹⁹ fuel cells,²⁰ photoreceptors,²¹ electronic packaging,²² authentication system for secure documents,²³ inks,^{24,25} correction fluid,²⁶ paints,²⁷ detection of defects in films,²⁸ floor coatings,²⁹ textiles,³⁰ corrosion testing,³¹ explosive,³² concrete,³³ toys,³⁴ detecting lipase activity of crop seeds,³⁵ soaps,³⁶ method for prevention of drug misuse,³⁷ cosmetics,³⁸ diapers,³⁹ detecting viable cells,⁴⁰ carbohydrates,⁴¹ antimalarial,⁴² antibacterial,⁴³ treating amyloid-associated diseases⁴⁴

Safety/Toxicity Bacterial toxicity,⁴⁵ ovarian cancer risk,⁴⁶ carcinogenicity,^{47–53} genotoxicity,^{53–56} mutagenicity,⁵⁷ toxicokinetics,⁵⁸ chromosomal aberration^{59,60}

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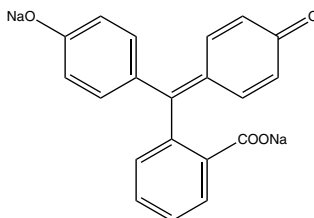
PHENOLPHTHALEIN, DISODIUM SALT

Other Names Phenolphthalein, disodium salt; Phenolphthalein sodium

CA Index Name 1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxyphenyl)-, disodium salt

CAS Registry Number 518-51-4

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Phthalein

Molecular Formula $C_{20}H_{12}O_4Na_2$

Molecular Weight 362.29

pH Range 8.0–10.0

Color Change at pH Colorless (8.0) to pink (10.0)

pKa 9.1

Physical Form Dark red powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 553 nm

Melting Point >250°C

Synthesis Synthetic method^{1–3}

Major Applications Inks,⁴ fire-resistant polymers,⁵ permanent hair straightener⁶

Safety/Toxicity No data available

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PHENOL RED

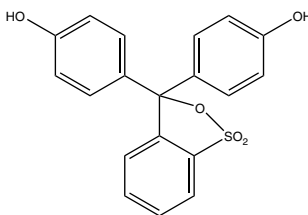
Other Names Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)*bis*-, *S,S*-dioxide; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)di-, *S,S*-dioxide; 3H-2,1-Benzoxathiole, phenol deriv.; α -Hydroxy- α,α -*bis*(*p*-hydroxyphenyl)-*o*-toluenesulfonic acid γ -sultone; 3,3-*Bis*(*p*-hydroxyphenyl)-2,1,3H-benzoxathiole 1,1-dioxide; 3H-2,1-Benzoxathiole, 3,3-*bis*(4-hydroxyphenyl)-, 1,1-dioxide; Fenolipuna; NSC 10459; PSP; PSP (indicator); Phenol red; Phenolsulfonephthalein; Phenolsulfonphthalein; Phenolsulphonphthalein; Sulfonphthal; Sulphental; Sulphonthal; TF-R 2

CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)*bis*-

CAS Registry Number 143-74-8

Merck Index Number 7247

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula C₁₉H₁₄O₅S

Molecular Weight 354.38

pH Range 6.8–8.4

Color Change at pH Yellow (6.8) to red (8.4)

pKa 7.90

Physical Form Red crystals

Solubility Sparingly soluble in water; soluble in ethanol; almost insoluble in ether, chloroform

UV-Visible (λ_{max}) 557 nm, 558 nm, 360 nm, 423 nm, 433 nm

Melting Point >300°C

Boiling Point (Calcd.) 562.8 $\pm$ 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods¹⁻⁶

Major Applications Display device,⁷ sol-gel matrix,⁸ photoreceptors,⁹ fuel cells,¹⁰ waveguides,¹¹ paints,¹² detergents,¹³ cosmetics,¹⁴ antiperspirant composition,¹⁵ diapers,¹⁶ screening bacteria,¹⁷ detecting viable cells,¹⁸ diagnosis of urogenital ureaplasmosis,¹⁹ treatment of pathogen infections,²⁰ amyloid-associated diseases,²¹ glaucoma,²² pulmonary hypertension,²² asthma,²² chronic obstructive pulmonary disease,²² erectile dysfunction,²² Raynaud's syndrome,²² heparin overdose,²² vulvodynia,²² wound healing,²² psychoactive drugs,²³ evaluating dental caries activity²⁴

Safety/Toxicity Carcinogenicity,²⁵ environmental analysis,²⁶ dye-induced cholestasis,²⁷ mutagenicity,²⁸ Nephrotoxicity^{29,30}

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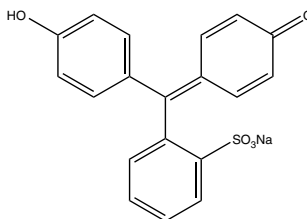
PHENOL RED, SODIUM SALT

Other Names Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)*bis*-, *S,S*-dioxide, monosodium salt; 3H-2,1-Benzoxathiole, phenol deriv.; Phenol red sodium; Phenol red, sodium salt; Phenolsulfonephthalein sodium

CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)*bis*-, monosodium salt

CAS Registry Number 34487-61-1

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Sulfonephthalein

Molecular Formula C₁₉H₁₃O₅SNa

Molecular Weight 376.36

pH Range 6.8–8.4

Color Change at pH Yellow (6.8) to red (8.4)

pKa 7.69, 7.9, 1.3

Physical Form Shiny dark-red crystals

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 423 nm, 557 nm

Melting Point 285°C

Synthesis Synthetic method^{1–3}

Major Applications Sensor,⁴ optical device,⁵ paints,⁶ sterilization process,⁷ fertilizer,⁸ detecting viable cells,⁹ gastrointestinal mucosa,¹⁰ antibacterial agent,¹¹ drugs,¹² pharmacology¹³

Safety/Toxicity Toxic blocking activity¹³

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4-(PHENYLAZO)-DIPHENYLAMINE

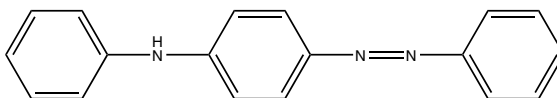
Other Names Diphenylamine, 4-(phenylazo)-; 4-(Phenylamino)azobenzene; 4- (Phenylazo)diphenylamine; 4-Anilinoazobenzene; 4- Phenazodiphenylamine; *N*-Phenyl-4-(phenylazo)aniline; *N*- Phenyl-4-(phenylazo)benzenamine; *N*-Phenyl-4-aminoazobenzene; NSC 74774

CA Index Name Benzenamine, *N*-phenyl-4-(phenylazo)-

CAS Registry Number 101-75-7

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula C₁₈H₁₅N₃

Molecular Weight 273.33

pH Range 1.2–2.5

Color Change at pH Red (1.2) to yellow (2.5)

pKa 0.42

Physical Form Orange powder

Solubility Insoluble in water; soluble in ethanol, methanol

UV-Visible (λ_{max}) 411 nm, 272 nm

Melting Point 89–91°C

Boiling Point (Calcd.) 451.7 ± 28.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–12}

Major Applications Display device,¹³ nonlinear optical (NLO) material,¹⁴ photoresists,¹⁵ printing plates,^{16,17} lithographic plates,¹⁸ photosensitive materials,¹⁹ photography,²⁰ markers²¹

Safety/Toxicity Oral toxicity²²

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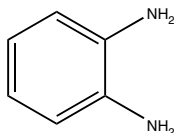
o-PHENYLENEDIAMINE

Other Names *o*-Phenylenediamine; 1,2-Diaminobenzene; 1,2-Phenylenediamine; 2-Aminoaniline; C.I. 76010; C.I. Oxidation Base 16; IK 3; IK 3 (amine); NSC 5354; Orthamine; *o*-Aminoaniline; *o*-Aminophenylamine; *o*-Benzenediamine; *o*-Diaminobenzene

CA Index Name 1,2-Benzenediamine

CAS Registry Number 95-54-5

Merck Index Number 7284

Chemical Structure

Chemical/Dye Class Fluorescent

Molecular Formula C₆H₈N₂

Molecular Weight 108.14

pH Range 3.1–4.4

Color Change at pH Green fluorescence (3.1) to nonfluorescence (4.4)

pKa 4.46

Physical Form Brown crystals

Solubility Slightly soluble in water; freely soluble in ethanol, ether, chloroform

Melting Point 103–104°C

Boiling Point 256–258°C

Synthesis Synthetic methods^{1–8}

Major Applications Bottom antireflective coatings,⁹ semiconductor devices,¹⁰ hair dyes,¹¹ detecting antibody,¹² glucose,¹³ streptomycin,¹⁴ penicillin,¹⁵ sulfonamide,¹⁶ neuroglobin,¹⁷ substrate for horse radish peroxidase¹⁸

Safety/Toxicity Acute toxicity,¹⁹ aquatic toxicity,²⁰ carcinogenicity,²¹ chemical toxicity,²² hepatotoxicity,²³ cytotoxicity,²³ genotoxicity,²⁴ mutagenicity,^{25,26} oral toxicity,²⁷ percutaneous toxicity,²⁸ phytotoxicity²⁹

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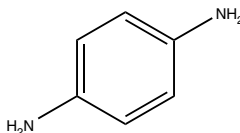
***p*-PHENYLENEDIAMINE**

OtherNames *p*-Phenylenediamine; 1,4-Diaminobenzene; 1,4-Diaminobenzol; 1,4-Phenylenediamine; 4-Aminoaniline; BASF Ursol D; Benzofur D; Black for Fur D; C.I. 76060; C.I. Developer 13; C.I. Oxidation Base 10; Developer PF; Durafur Black R; Fouramine D; Fournine 1; Fournine D; Fur Black 41867; Fur Brown 41866; Fur Yellow; Furro D; Futramine D; NSC 4777; Nako H; Orsin; PPD; Pelagol D; Pelagol DR; Pelagol Grey D; Peltol D; Renal PF; Rodol DJ; Tertral D; Ursol D; Zoba Black D; *p*-Aminoaniline; *p*-Benzenediamine; *p*-Diaminobenzene

CA Index Name 1,4-Benzenediamine

CAS Registry Number 106-50-3

Merck Index Number 7285

Chemical Structure

Chemical/Dye Class Fluorescent

Molecular Formula C₆H₈N₂

Molecular Weight 108.14

pH Range 3.1–4.4

Color Change at pH Nonfluorescence (3.1) to orange/yellow fluorescence (4.4)

pKa 4.17

Physical Form White to slightly red crystals, darkens on exposure to air

Solubility Slightly soluble in water; soluble in ethanol, ether, chloroform

Melting Point 145–147°C

Boiling Point 267°C

Synthesis Synthetic methods^{1–10}

Major Applications Nanoparticles,¹¹ liquid crystal displays,¹² chemical mechanical polishing,¹³ bottom antireflective coatings,¹⁴ electrochromic materials,¹⁵ inks,¹⁶ rubber,¹⁷ hair dyes,¹⁸ cosmetics,¹⁹ treatment of virus skin infection²⁰

Safety/Toxicity Acute toxicity,²¹ cytotoxicity,²¹ carcinogenicity,²² genotoxicity,²³ mutagenicity²⁴

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PHLOXINE B

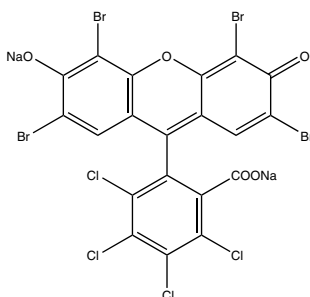
Other Names Fluorescein, 2',4',5',7'-tetrabromo-4,5,6,7-tetrachloro-, disodium salt; 11969 Red; 3427 Veri Pur Pink; Acid Red 92; Aizen Acid Phloxine PB; C.I. 45410; C.I. Acid Red 92; Cyanosin; Cyanosin (acid dye); Cyanosin B; Cyanosine; D and C Red No. 28; D&C Red 28; D&C Red No. 28; Daiwa Red 104WB; Daiwa Red 45; Disodium 9-(3',4',5',6'-tetrachloro-*o*-carboxyphenyl)-6-hydroxy-6-hydroxy-2,4,5,7-tetrabromo-3-isoxanthone; Eosin blue; Eosin bluish; Eosine blue; Eosine bluish; Food Red 104; Food Red No. 104; Japan Red 104; Japan Red 104-1; Orient Water Pink 2; Phloxine B; Phloxine P; Phyloxine B; Red 104; Red No. 104; Red No.104-1; Water Pink 2

CA Index Name Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 2',4',5',7'-tetrabromo-4,5,6,7-tetrachloro-3',6'-dihydroxy-, disodium salt

CAS Registry Number 18472-87-2

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Xanthene, Fluorescent

Molecular Formula C₂₀H₂Br₄Cl₄O₅Na₂

Molecular Weight 829.66

pH Range 2.5–4.0

Color Change at pH Nonfluorescence (2.5) to yellowish-blue fluorescence (4.0)

Physical Form Brick-red powder

Solubility Soluble in water, ethylene glycol; slightly soluble in ethanol, methanol

UV-Visible (λ_{max}) 548 nm, 510 nm

Melting Point >250°C

Synthesis Synthetic methods^{1–6}

Major Applications Optical waveguides,⁷ color filter,⁸ lithographic printing plates,⁹ display device,¹⁰ inks,^{11–13} highlighters,¹⁴ textiles,¹⁵ hair dyes,¹⁶ cosmetics,^{17–19} visualization of dental plaque,²⁰ treatment of infectitious diseases,²¹ antitumor agents²²

Safety/Toxicity Acute and chronic toxicity,²³ cytotoxicity,²⁴ estrogenicity,²⁵ eye irritation tests,²⁶ toxicity to insects,²⁷ mutagenicity,²⁸ oral toxicity,²⁹ phototoxicity,³⁰ teratogenicity,³¹ topical toxicity³²

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PICRIC ACID

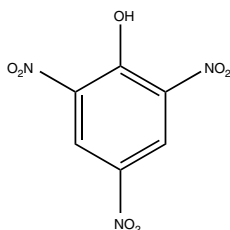
Other Names Picric acid; 1-Hydroxy-2,4,6-trinitrobenzene; 2,4,6-Trinitrophenol; C.I. 10305; Carbazotic acid; Melinite; NSC 36947; NSC 56147; Nitroxanthic acid; PA; Picral; Picronitric acid; Trinitrophenol

CA Index Name Phenol, 2,4,6-trinitro-

CAS Registry Number 88-89-1

Merck Index Number 7410

Chemical Structure



Chemical/Dye Class Nitro

Molecular Formula $C_6H_3N_3O_7$

Molecular Weight 229.10

pH Range 0.0–1.3

Color Change at pH Colorless (0.0) to yellow (1.3)

pKa 0.53

Physical Form Pale yellow glittering crystals

Solubility Soluble in water, ethanol, benzene, chloroform; insoluble in toluene

UV-Visible (λ_{max}) 354 nm

Melting Point 122–123°C

Boiling Point (Calcd.) $303.6 \pm 42.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods^{1–8}

Major Applications Explosives,⁹ power circuits,¹⁰ energetic materials,¹¹ liquefied gas fuels,¹² thin films,¹³ power generation,¹⁴ batteries,^{14,15} fuel cells,¹⁶ steel,¹⁷ gold films,¹⁸ nanopowder,¹⁹ antifreeze fluid for automobiles,²⁰ polymerization inhibitors,²¹ tattoo removal from skin,²² antiinflammatory agent,²³ treatment of neoplasm²⁴

Safety/Toxicity Acute toxicity,^{25,26} algal toxicity,^{27,28} toxicity to aquatic organisms,²⁹ toxicity to bacteria,³⁰ ecotoxicity,³¹ environmental pollutants,³² genotoxicity,³³ marine toxicity,³⁴ mutagenicity,³⁵ neurotoxicity³⁶

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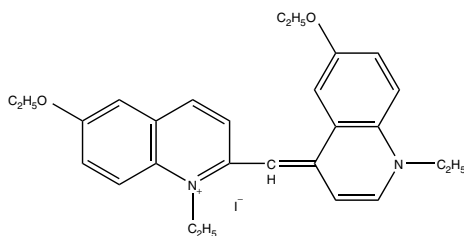
PINACHROME

Other Names Quinolinium, 6-ethoxy-2-[(6-ethoxy-1-ethyl-4(1H)-quinolyldiene)-methyl]-1-ethyl, iodide; Pinachrome; Pinachrome NK 914

CA Index Name Quinolinium, 6-ethoxy-2-[(6-ethoxy-1-ethyl-4(1H)-quinolinylidene)methyl]-1-ethyl-, iodide

CAS Registry Number 27593-93-7

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Quinoline

Molecular Formula $C_{27}H_{31}N_2O_2I$

Molecular Weight 518

pH Range 5.6–8.0

Color Change at pH Colorless (5.6) to red-violet (8.0)

pKa 7.34

Physical Form Dark green powder

Solubility Soluble in water, ethanol, dilute hydrochloric acid (most commonly used)

Melting Point $>250^{\circ}\text{C}$

Synthesis Synthetic method¹

Major Applications Inks,² dichromated gelatin,³ photographic sensitizer⁴

Safety/Toxicity No data available

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POIRRIER BLUE

Other Names Poarie Blue C 4B
CA Index Name Poirrier Blue C 4B
CAS Registry Number 1400-96-0
Merck Index Number Not listed
Chemical Structure No structure diagram available
Chemical/Dye Class Triphenylmethane
Molecular Formula Unspecified
Molecular Weight Not available
pH Range 11.0–13.0
Color Change at pH Blue (11.0) to violet-red (13.0)
Physical Form Blue powder
Solubility Soluble in water, ethanol
Melting Point Not available
Synthesis Synthetic method¹
Major Applications detecting degradation of concrete²
Safety/Toxicity No data available

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P

PROPYL RED

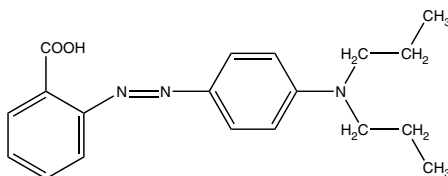
Other Names Benzoic acid, *o*-[[*p*-(dipropylamino)phenyl]azo]-; 2-[4-(Dipropylamino)phenylazo] benzoic acid; NSC 7803; Propyl red

CA Index Name Benzoic acid, 2-[[4-(dipropylamino)phenyl]azo]-

CAS Registry Number 2641-01-2

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula C₁₉H₂₃N₃O₂

Molecular Weight 325.40

pH Range 4.6–6.6

Color Change at pH Red (4.6) to yellow (6.6)

pKa 5.48

Physical Form Yellow-orange solid

Solubility Insoluble in water; soluble in ethanol, methanol

Melting Point >250°C

Boiling Point (Calcd.) 515.8 ± 35.0°C Pressure: 760 Torr

Synthesis Synthetic method¹

Major Applications Electrophoresis display device,² image contrast-enhancing layer,³ photography,⁴ Photoelectrographic imaging,⁵ inks,⁶ paints,⁶ toys⁶

Safety/Toxicity No data available

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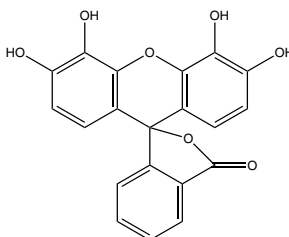
PYROGALLOLPHTHALEIN

Other Names Gallein; Alizarine violet; C.I. 45445; C.I. Mordant Violet 25; Mordant Violet 25; NSC 56445; NSC 622478; NSC 8668; Pyrogallolphthalein

CA Index Name Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',4',5',6'-tetrahydroxy-

CAS Registry Number 2103-64-2

Merck Index Number 4344

Chemical Structure

Chemical/Dye Class Miscellaneous, Xanthene

Molecular Formula C₂₀H₁₂O₇

Molecular Weight 364.31

pH Range 3.8–6.6;

10.6–13.0

Color Change at pH Yellow (3.8) to rose-red (6.6)

Pink (10.6) to violet (13.0)

pKa 5.99

Physical Form Brownish-red powder

Solubility Almost insoluble in water, benzene, chloroform; soluble in ethanol, acetone

Melting Point >300°C

Boiling Point (Calcd.) 687.4 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–7}

Major Applications Organic light emitting devices (OLED),⁸ semiconductors,^{9,10} photoresists,^{11,12} lithographic printing plates,¹³ method for ozone determination,¹⁴ treatment of wastewater,¹⁵ determination of silver,¹⁶ nail polish,¹⁷ monitoring sterilization,¹⁸ determination of proteins,¹⁹ induce apoptosis in cancer cells,²⁰ treatment of cancer cells,²¹ antiHIV agent,²² diagnosis and treatment of amyloidosis,²³ cancer chemopreventive activity,²⁴ drug design,²⁵ inhibition of influenza virus²⁶

Safety/Toxicity No data available

References

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Q

QUINALDINE RED

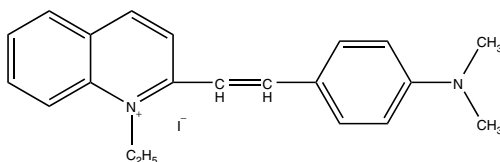
Other Names 2-[*p*-(Dimethylamino)styryl]-1-ethylquinolinium iodide; Quinaldine Red; Quinolinium, 2-[*p*-(dimethylamino)styryl]-1-ethyl-, iodide; α -(*p*-Dimethylaminophenylethylene) quinoline ethiodide; 1-Ethyl-2-(*p*-dimethylaminostyryl)quinoline iodide; 2-(*p*-Dimethylaminostyryl) quinoline ethiodide; 2-[4-(Dimethylamino)styryl]-1-ethylquinolinium iodide; Eastman 1361

CA Index Name Quinolinium, 2-[2-[4-(dimethylamino)phenyl]ethenyl]-1-ethyl-, iodide

CAS Registry Number 117-92-0

Merck Index Number 8049

Chemical Structure



Chemical/Dye Class Miscellaneous, Quinoline, Styryl

Molecular Formula $C_{21}H_{23}N_2I$

Molecular Weight 430.33

pH Range 1.4–3.2

Color Change at pH Colorless (1.4) to red (3.2)

pKa 2.63

Physical Form Very dark red or reddish-black powder

Solubility Sparingly soluble in water; freely soluble in ethanol

UV-Visible (λ_{max}) 528 nm

Melting Point 241–243°C

Synthesis Synthetic methods^{1–4}

Major Applications Display device,^{5,6} photoresists,⁷ lithographic plates,^{8,9} toner,¹⁰ paints,¹¹ coating materials,¹² hair dye,¹³ treatment of mechanical allodynia,¹⁴ regulation of cell proliferation,¹⁵ diagnostic agents for diseases related with amyloid accumulation,¹⁶ treatment of virus infectious diseases,¹⁷ detecting enzyme activity,¹⁸ dental bleaching materials¹⁹

Safety/Toxicity No data available

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QUININE

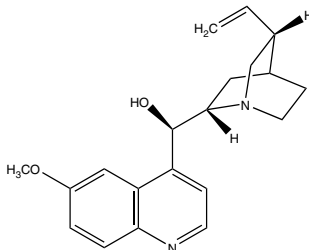
Other Names Quinine; (–)-Quinine; (8S,9R)-Quinine; (R)-(–)-Quinine; 6'-Methoxycinchonidine; Chinine; NSC 192949

CA Index Name Cinchonan-9-ol, 6'-methoxy-, (8 α ,9R)-

CAS Registry Number 130-95-0

Merck Index Number 8061

Chemical Structure



Chemical/Dye Class Fluorescent, Quinoline

Molecular Formula C₂₀H₂₄N₂O₂

Molecular Weight 324.42

pH Range 3.0–5.0;
9.5–10.0

Color Change at pH Blue fluorescence (3.0) to weak violet fluorescence (5.0)

Weak violet fluorescence (9.5) to nonfluorescence (10.0)

pKa 5.07, 9.7

Physical Form White to off-white powder

Solubility Slightly soluble in water; soluble in ethanol, chloroform, glycerol; insoluble in petroleum ether

Melting Point 177°C (decompose)

Boiling Point 495.9 ± 40.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–5}

Major Applications Bird repellents,⁶ sunscreen,⁷ antimalarial agent,⁸ antiviral agent,^{9,10} antitumor agent,¹¹ antiparasitic agent,¹¹ treatment of epilepsy,¹² skeletal muscle spasm,¹³ drug-coated coronary stent system¹⁴

Safety/Toxicity Antimalarial drug toxicity,¹⁵ cardiotoxicity,¹⁶ cytotoxicity,¹⁷ hepatotoxicity,¹⁷ human toxicity,¹⁸ ototoxicity,¹⁹ phototoxicity²⁰

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QUININIC ACID

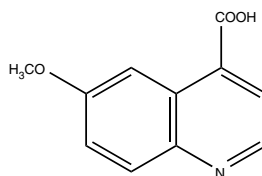
Other Names Cinchoninic acid, 6-methoxy-; 6-Methoxy-4-quinolinecarboxylic acid; 6-Methoxy-cinchoninic acid; NSC 403610; Quininic acid

CA Index Name 4-Quinolinecarboxylic acid, 6-methoxy-

CAS Registry Number 86-68-0

Merck Index Number 8062

Chemical Structure



Chemical/Dye Class Fluorescent, Quinoline

Molecular Formula C₁₁H₉NO₃

Molecular Weight 203.19

pH Range 4.0–5.0

Color Change at pH Yellow fluorescent (4.0) to blue fluorescent (5.0)

pKa 5.53

Physical Form Pale yellow crystals

Solubility Slightly soluble in water, cold ethanol, ether

Melting Point 280°C (decompose)

Boiling Point (Calcd.) 385.4 ± 22.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–9}

Major Applications Display device,¹⁰ antihypertensive food materials,¹¹ nucleic acids,¹² antibacterial agent,^{1–7} antimalarial agent⁹

Safety/Toxicity No data available

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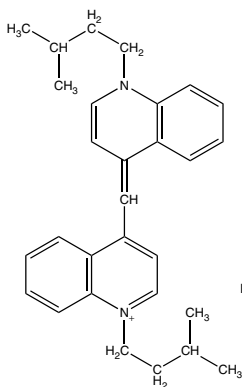
QUINOLINE BLUE

OtherNames 1-Isopentyl-4-[(1-isopentyl-4(1H)-quinolylidene)methyl]-quinoliniumiodide; Cyanine blue; Quinolinium, 1-isopentyl-4-[(1-isopentyl-4(1H)-quinolylidene)methyl]-, iodide; Aquafine Blue E 1; Chinoline blue; Cyanine; Cyanine Blue 4920; Cyanine Blue GR; NK 1486; Quinoline blue
CA Index Name Quinolinium, 1-(3-methylbutyl)-4-[[1-(3-methylbutyl)-4(1H)-quinolinylidene]methyl]-, iodide

CAS Registry Number 523-42-2

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Quinoline

Molecular Formula C₂₉H₃₅N₂I

Molecular Weight 538.50

pH Range 7.0–8.0

Color Change at pH Colorless (7.0) to blue-violet (8.0)

Physical Form Green needles or crystals with dark lustre

Solubility Sparingly soluble in hot water; soluble in ethanol

Melting Point >250°C

Synthesis Synthetic methods^{1,2}

Major Applications Display device,³ semiconductors,^{4,5} optical fibers,⁶ antireflection films,⁷ photoimaging process,⁸ printed circuit board,⁹ inks,^{10–12} toners,^{13,14} paints,^{15,16} adhesives,^{17,18} packing materials,¹⁹ molding materials for fiber-reinforced plastics,²⁰ building materials,²¹ prediction of deterioration of resins,²² materials for treating animal manure²³

Safety/Toxicity Environmental pollutants²⁴

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R

RESAZURIN

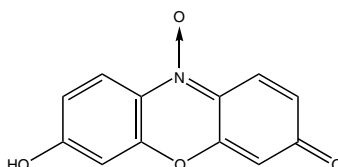
Other Names Resazurin; 7-Hydroxy-3H-phenoxazin-3-one 10-oxide; 7-Hydroxy-3H-phenoxazine-3-one 10-oxide; Alamar Blue; Azoresorcin; Diazaresorcinol; NSC 10438; NSC 56323; Resazoin; Resazurine; Rhodalux

CA Index Name 3H-Phenoxazin-3-one, 7-hydroxy-, 10-oxide

CAS Registry Number 550-82-3

Merck Index Number 8141

Chemical Structure



Chemical/Dye Class Miscellaneous, Oxazone, Heterocyclic

Molecular Formula C₁₂H₇NO₄

Molecular Weight 229.19

pH Range 3.8–6.5

Color Change at pH Orange (3.8) to purple-violet (6.5)

pKa 6.71

Physical Form Dark red crystals with greenish luster

Solubility Insoluble in water, ether; sparingly soluble in ethanol

UV-Visible (λ_{max}) 598 nm, 380 nm

Melting Point >250°C

Boiling Point (Calcd.) 477.2 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Display device,³ inks,⁴ detergents,⁵ analysis of soil samples,⁶ cosmetics,⁷ measuring freshness of fruit,⁸ sorbitol,⁹ monitoring sugar loss,¹⁰ assessment of microbials,¹¹ assays for cells,¹² mitochondria,¹³ semen quality,¹⁴ detecting antiviral substances,¹⁵ diagnosis of bacterial and fungal infection,¹⁶ treating pulmonary tuberculosis,¹⁷ oral care formulation¹⁸

Safety/Toxicity Cytotoxicity,¹⁹ chemical toxicity,²⁰ hepatotoxicity,²¹ nephrotoxicity²²

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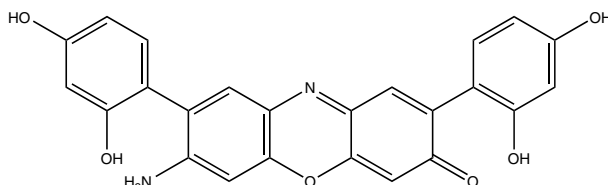
RESORCEIN

OtherNames 2-Amino-3,6-bis(2,4-dihydroxyphenyl)-2-phenoxazone; Fluorescent Blue; Iris Blue B; Lacmoid; Resorcein; Resorcein Blue

CA Index Name 3H-Phenoxazin-3-one, 7-amino-2,8-bis(2,4-dihydroxyphenyl)-

CAS Registry Number 33869-21-5

Merck Index Number 5332

Chemical Structure

Chemical/Dye Class Miscellaneous

Molecular Formula C₂₄H₁₆N₂O₆

Molecular Weight 428.39

pH Range 4.4–6.4

Color Change at pH Red (4.4) to blue (6.4)

pKa 5.31

Physical Form Black-violet powder

Solubility Sparingly soluble in water, ether; soluble in ethanol, methanol, amyl alcohol, acetone, acetic acid; practically insoluble in chloroform, benzene, petroleum ether

UV-Visible (λ_{max}) 611 nm

Melting Point >250°C

Boiling Point (Calcd.) 755.3 ± 60.0°C Pressure: 760

Synthesis Synthetic methods^{1–3}

Major Applications Electrochromic devices,⁴ photosensitive materials,⁵ parasiticides,⁶ hair dyes,⁷ cosmetics,⁸ ointment for hemorrhoids⁹

Safety/Toxicity Fish toxicity¹⁰

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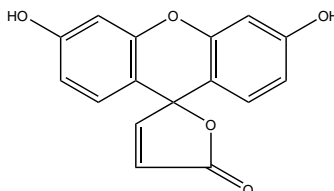
RESORCINMALEIN

Other Names Spiro[furan-2(5H),9'-xanthen]-5-one, 3',6'-dihydroxy-; Xanthene-9-acrylic acid, 3,6,9-trihydroxy-, γ -lactone; NSC 119894; Resorcinolmalein

CA Index Name Spiro[furan-2(5H),9'-[9H]xanthen]-5-one, 3',6'-dihydroxy-

CAS Registry Number 1227-88-9

Merck Index Number Not listed

Chemical Structure**R**

Chemical/Dye Class Miscellaneous

Molecular Formula C₁₆H₁₀O₅

Molecular Weight 282.25

pH Range 5.0–6.5

Color Change at pH Yellow (5.0) to orange-red (6.5)

pKa 5.66

Physical Form Yellow crystals

Solubility Insoluble in water, soluble in ethanol, acetone

Melting Point 275–276°C

Boiling Point (Calcd.) 610.5 $\pm$ 55.0°C Pressure: 760 Torr

Synthesis Synthetic methods¹

Major Applications Toner,² antiHIV agent³

Safety/Toxicity No data available

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RESORUFIN

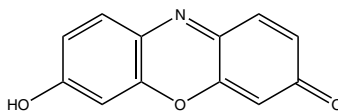
Other Names Resorufin; 7-Hydroxy-3H-phenoxazin-3-one; 7-Hydroxyphenoxazin-3-one; 7-Hydroxyphenoxazin-3-one; NSC 12097; Resorufine

CA Index Name 3H-Phenoxazin-3-one, 7-hydroxy-

CAS Registry Number 635-78-9

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent, Oxazone, Heterocyclic

Molecular Formula C₁₂H₇NO₃

Molecular Weight 213.19

pH Range 4.4–6.4

Color Change at pH Yellow fluorescent (4.4) to orange fluorescent (6.4)

pKa 6.6

Physical Form Purple powder

Solubility Sparingly soluble in water; soluble in ethanol, *N,N*-dimethylformamide

UV-Visible (λ_{max}) 573 nm, 571 nm, 585 nm, 480 nm

Melting Point >300°C

Boiling Point (Calcd.) 413.0 ± 45.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–4}

Major Applications Photoelectrochemical cells,⁵ electrochromic devices,⁶ display device,⁷ inks,⁸ redox indicator,⁹ oil product detection,¹⁰ dye laser,¹¹ chemiluminescence detection,¹² cosmetics,¹³ microbial fuel cells,¹⁴ cytochrome P 450 assay,¹⁵ multiplex assays,¹⁶ analyzing cells,¹⁷ semen quality,¹⁸ testing prenatal abnormalities,¹⁹ detecting nucleic acids,²⁰ antitumor agent²¹

Safety/Toxicity Toxicity,²² mutagenicity²³

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RHODOL GREEN

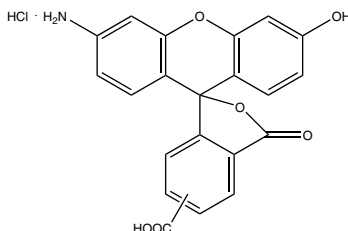
Other Names Rhodol Green carboxylic acid, hydrochloride 5(6)-CRF 492

CA Index Name Rhodol Green

CAS Registry Number 183185-51-5

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula $C_{21}H_{14}ClNO_6$

Molecular Weight 411.80

pH Range 5.0–7.8

Color Change at pH Weak green fluorescence (5.0) to strong green fluorescence (7.8)

pKa 5.6

Physical Form Solid

Solubility Insoluble in water; soluble in *N,N*-dimethylformamide

UV-Visible (λ_{max}) 480 nm

Melting Point >250°C

Synthesis Synthetic method¹

Major Applications Optical sensors,² determining the size of polynucleotides,³ diagnosis of parathyroid carcinoma,⁴ genetic diseases,⁵ detecting multiple nucleic acid targets,⁶ antitumor agent⁷

Safety/Toxicity No data available

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p-ROSOLIC ACID

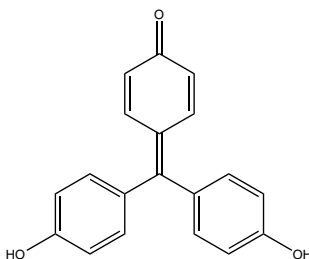
Other Names 2,5-Cyclohexadien-1-one, 4-[bis(p-hydroxyphenyl)methylene]-; Aurin; 4,4'-Dihydroxyfuchson; 4-(p,p'-Dihydroxybenzhydrylidene)-2,5-cyclohexadien-1-one; 4-[Bis(p-hydroxyphenyl)methylene]-2,5-cyclohexadien-1-one; Aurin 555; Aurine; C.I. 43800; Corallin; Corallin Spirit Soluble; NSC 7805; Pararosolic acid; Rosalic acid; Spirit Aurine; p-Rosolic acid

CA Index Name 2,5-Cyclohexadien-1-one, 4-[bis(4-hydroxyphenyl)methylene]-

CAS Registry Number 603-45-2

Merck Index Number 881

Chemical Structure



Chemical/Dye Class Triphenylmethane

Molecular Formula C₁₉H₁₄O₃

Molecular Weight 290.31

pH Range 6.6–8.0

Color Change at pH Yellow (6.6) to red (8.0)

pKa 6.98

Physical Form Red crystals

Solubility Practically insoluble in water, benzene; freely soluble in ethanol

UV-Visible (λ_{max}) 534.6 nm, 479.5 nm, 482 nm

Melting Point 309°C (decompose)

Boiling Point (Calcd.) 543.0 ± 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–9}

Major Applications Antireflective coatings,¹⁰ thermochromic materials,¹¹ photoresists,² electrorheological materials,¹² film patterning,¹³ recording materials,¹⁴ lithium battery,¹⁵ semiconductors,¹⁶ printing materials,¹⁷ inks,¹⁸ corrosion inhibitors,¹⁹ adhesives,²⁰ drugs,²¹ detecting viable cells,²² treatment of Alzheimer's disease¹

Safety/Toxicity Toxic activity,²³ environmental toxicity,²⁴ cytopathogenicity²⁵

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RUBROPHEN

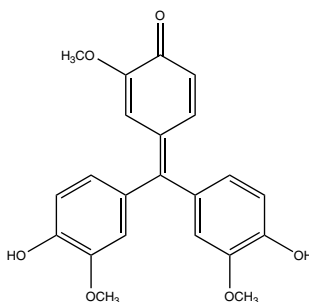
Other Names Rubrophen; NSC 71806; Rubrocol

CA Index Name 2,5-Cyclohexadien-1-one, 4-[bis(4-hydroxy-3-methoxyphenyl)-methylene]-2-methoxy-

CAS Registry Number 5664-34-6

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Triphenylmethane

Molecular Formula C₂₂H₂₀O₆

Molecular Weight 380.39

pH Range 1.0–3.0;

6.5–7.2

Color Change at pH Cherry-red (1.0) to yellow (3.0)

Yellow (6.5) to violet (7.2)

pKa 3.0, 4.4, 10.0

Physical Form Solid

Solubility Slightly soluble in water; soluble in ethanol

Melting Point 251°C

Boiling Point (Calcd.) 646.1 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–7}

Major Applications Pharmaceutical,⁸ fungicides,⁹ treatment of tuberculosis¹⁰

Safety/Toxicity No data available

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S

SALICYLALDEHYDE SEMICARBAZONE

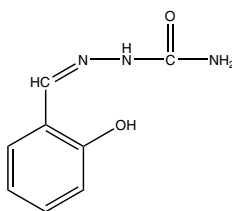
Other Names Salicylaldehyde, semicarbazone; 2-Hydroxybenzaldehyde semicarbazone; NSC 1604

CA Index Name Hydrazinecarboxamide, 2-[(2-hydroxyphenyl)methylene]-

CAS Registry Number 3030-97-5

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula C₈H₉N₃O₂

Molecular Weight 179.18

pH Range 7.6–8.0

Color Change at pH Yellow fluorescence (7.6) to blue fluorescence (8.0)

pKa 7.75

Physical Form Solid

Solubility Insoluble in water; soluble in ethanol

Melting Point 227–228°C

Synthesis Synthetic methods^{1–5}

Major Applications Electroluminescent devices,⁶ semiconductor wafer,⁷ corrosion inhibitors,⁸ antibacterial agent,¹ anticonvulsant agent,⁹ anticancer agent¹⁰

Safety/Toxicity No data available

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SALICYLIC ACID

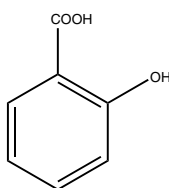
Other Names 171; 2-Carboxyphenol; 2-Hydroxybenzenecarboxylic acid; 2-Hydroxybenzoic acid; 311; 334; 337; 380; 51; Advanced Pain Relief Callus Removers; Advanced Pain Relief Corn Removers; Clear away Wart Remover; Compound W; Dr. Scholl's Callus Removers; Dr. Scholl's Corn Removers; Dr. Scholl's Wart Remover Kit; Duofil Wart Remover; Duoplant; Freezone; Ionil; Ionil Plus; K 537; K 557; NSC 180; Phenol-2-carboxylic acid; Psoriacid-S-Stift; Retarder W; Rutranex; Salicylic Acid Soap; Salicylic acid collodion; Saligel; Salonil; Stri-Dex; Trans-Ver-Sal; *o*-Carboxyphenol; *o*-Hydroxybenzoic acid

CA Index Name Benzoic acid, 2-hydroxy-

CAS Registry Number 69-72-7

Merck Index Number 8332

Chemical Structure



Chemical/Dye Class Fluorescent

Molecular Formula C₇H₆O₃

Molecular Weight 138.12

pH Range 2.5–4.0

Color Change at pH Nonfluorescence (2.5) to dark blue fluorescence (4.0)

pKa 2.98

Physical Form White crystals

Solubility Slightly soluble in water; soluble in ethanol, acetone

UV-Visible (λ_{max}) 210 nm, 234 nm, 303 nm

Melting Point 159°C

Boiling Point 211°C

Synthesis Synthetic methods^{1–5}

Major Applications Semiconductors,^{6,7} nanoparticles,⁸ photoresists,⁹ lubricating oils,¹⁰ UV absorbers,¹¹ adhesive,¹² leather,¹³ cleaner,¹⁴ hair dye,¹⁵ soaps,¹⁶ cosmetics,¹⁷ pain medication,¹⁸ analgesics,¹⁹ antibacterial agent,²⁰ treatment of dandruff,²¹ hyperpigmented skin,²² tinea pedis,²³ onychomycosis,²⁴ osteoporosis,²⁵ beriberi,²⁶ fungicidal skin disease,²⁷ autoimmune disease²⁸

Safety/Toxicity Acute toxicity,²⁹ aquatic toxicity,³⁰ carcinogenicity,³¹ cytotoxicity,³² ecotoxicity,³³ environmental toxicity,³⁴ hemotoxicology,³⁵ mutagenicity,³⁶ safety assessment³⁷

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SALICYL YELLOW

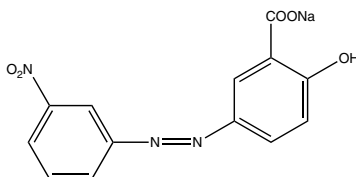
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CA Index Name Benzoic acid, 2-hydroxy-5-[(3-nitrophenyl)azo]-, monosodium salt

CAS Registry Number 584-42-9

Merck Index Number 5919

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula $C_{13}H_8N_3O_5Na$

Molecular Weight 309.22

pH Range 10.0–12.0

Color Change at pH Yellow (10.0) to orange (12.0)

Physical Form Yellow-orange powder

Solubility Soluble in water, methyl cellosolve; slightly soluble in ethanol, acetone

UV-Visible (λ_{max}) 362 nm

Melting Point >250°C

Synthesis Synthetic methods^{1–3}

Major Applications Optical engineering applications,⁴ sensors,⁵ making masks,⁶ electrorheological materials,⁷ surface treatment of copper,⁸ coloring zinc,⁹ aluminum,¹⁰ corrosion testing,¹¹ adhesive,¹² lubricants,¹³ textiles,¹⁴ food storage,¹⁵ determine bacterial growth,¹⁶ pharmaceutical preparations¹⁷

Safety/Toxicity Mutagenicity¹⁸

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SOLOCHROME VIOLET RS

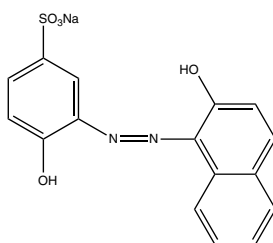
Other Names C.I. Mordant Violet 5; C.I. Mordant Violet 5, monosodium salt; Eriochrome Violet B; Acid Alizarin Violet N; Acid Alizarine Violet; Acid Alizarine Violet B; Acid Chrome Violet K; Acid Chrome Violet N; Aizen Chrome Violet BH; Alizarine Violet N; Alphacroic Violet B; Atlantichrome Violet B; Brasilan Chrome Violet B; C.I. 15670; Chromacid Violet R; Chromaven Violet B; Chrome Fast Violet B; Chrome Violet B; Chrome Violet K; Chrome Violet R; Cromal Violet B; Diacromo Violet N; Diamond Corinth N; Durochrome Violet B; Erio Chrome Violet BA; Erio Chrome Violet BR; Hispacrom Violet B; Java Chrome Violet B; Magracrom Violet N; Mitsui Chrome Violet BC; Monochrome Violet B; Mordant Violet 5; Omega Chrome Dark Violet D; Pontachrome Violet SW; Solochrome Violet; Solochrome Violet R; Solochrome Violet RS; Solocrom Violet RS; Sunchromine Violet B; Superchrome Violet B; Symulon Chrome Violet B; Tertrochrome Violet N; Yodochrome Violet B

CA Index Name Benzenesulfonic acid, 4-hydroxy-3-[(2-hydroxy-1-naphthalenyl)azo]-, monosodium salt

CAS Registry Number 2092-55-9

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula $C_{16}H_{11}N_2O_5SNa$

Molecular Weight 366.33

pH Range 6.5–9.0

Color Change at pH Orange-red (6.5) to violet (9.0)

pKa 4.35, 7.4, 9.35

Physical Form Reddish-violet crystals

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 501 nm

Melting Point >300°C

Synthesis Synthetic methods^{1–3}

Major Applications inks,⁴ dye lasers,⁵ in manufacture of vinyl polymers,⁶ textiles¹ determination of iron,⁷ calcium,⁸ aluminum,^{9–11} tantalum,¹² monitoring hardness in industrial water,¹³ measuring chlorine dioxide in drinking water,¹⁴ hypoglycemic agents,¹⁵ nuclear fluorochrome¹⁶

Safety/Toxicity Mutagenicity¹⁷

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SULPHAN BLUE

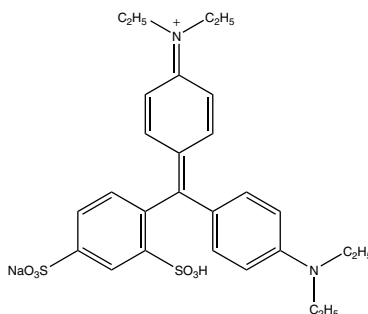
Other Names C.I. Acid Blue 1, sodium salt; Ethanaminium, *N*-[4-[[4-(diethylamino)phenyl](2,4-disulfophenyl)methylene]-2,5-cyclohexadien-1-ylidene]-*N*-ethyl-, hydroxide, inner salt, sodium salt; Xylene Blue VS; [4-[α -[*p*-(Diethylamino)phenyl]-2,4-isulfobenzylidene]-2,5-cyclohexadien-1-ylidene]-diethylammonium hydroxide, inner salt, sodium salt; 1085 Blue; Acid Blue 1; Acid Blue V; Acid Bright Azure Z; Acid Brilliant Blue Z; Acid Brilliant Sky Blue Z; Acid Leather Blue V; Acid Turquoise Blue V; Aizen Brilliant Acid Pure Blue VH; Alphazurine 2G; Amacid Blue V; Bleu Patente V; Blue URS; Blue VRS; Brilliant Acid Blue A Export; Brilliant Acid Blue V Extra; Brilliant Acid Blue VS; Brilliant Blue GS; Bucacid Patent Blue VF; C.I. 42045; C.I. Acid Blue 1; C.I. Food Blue 3; Carmine Blue VF; Disulfine blue VN; Disulphine Blue VN; Disulphine Blue VN 150; Disulphine VN; Duasyn Acid Blue V 02; Edicol Supra Blue VR; Erioglaurine supra; Fenazo Blue XF; Hexacol Blue VRS; Hidacid Blue V; Kiton Pure Blue V; Kiton Pure Blue V.FQ; Leather Blue G; Merantine Blue VF; Orient Water Blue 106; Patent Blue; Patent Blue V; Patent Blue VF; Patent Blue VF Special; Patent Blue VF-CF; Patent Pure Blue VX; Patent blue VS; Patent blue violet; Pontacyl Brilliant Blue V; Sodium Blue VRS; Sodium Patent Blue V; Sulfan blue; Sulphan Blue; Sumitomo Patent Pure Blue VX; Tertracid Carmine Blue V

CA Index Name Ethanaminium, *N*-[4-[[4-(diethylamino)phenyl](2,4-disulfophenyl)methylene]-2,5-cyclohexadien-1-ylidene]-*N*-ethyl-, inner salt, sodium salt

CAS Registry Number 129-17-9

Merck Index Number 8987

Chemical Structure



Chemical/Dye Class Triphenylmethane

Molecular Formula $C_{27}H_{31}N_2O_6S_2Na$

Molecular Weight 566.68

pH Range 0.8–3.0

Color Change at pH Yellow-orange (0.8) to deep blue (3.0)

Physical Form Dark blue powder

Solubility Soluble in water; partly soluble in ethanol; insoluble in xylene

UV-Visible (λ_{max}) 635 nm, 410 nm

Melting Point >250°C

Synthesis Synthetic methods¹⁻³

Major Applications Liquid crystal displays,⁴ color filters,^{5,6} electrorheological materials,⁷ photographic materials,⁸ optical filters,⁹ inks,¹⁰ highlighters,¹¹ dyeing paper,¹² wood dyeing,¹³ textiles,¹⁴ detergents,¹⁵ hair dyes,¹⁶ cosmetics,¹⁷ lymph node identification,¹⁸ antiparasitic agent,¹⁹ nanocomposite particles for biomedical applications²⁰

Safety/Toxicity Acute toxicity,²¹ genotoxicity,²² mutagenicity,^{23,24} allergic reaction,²⁵ adverse reaction²⁶

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TETRABROMOPHENOL BLUE

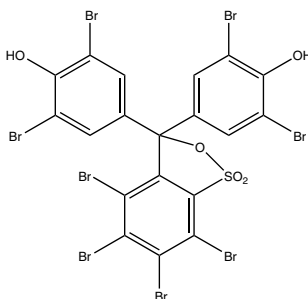
Other Names Phenol, 4,4'-(4,5,6,7-tetrabromo-3H-2,1-benzoxathiol-3-ylidene)-bis[2,6-dibromo-, S,S-dioxide; 3H-2,1-Benzoxathiole, phenol derivative; NSC 11236; Tetrabromophenol blue

CA Index Name Phenol, 4,4'-(4,5,6,7-tetrabromo-1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dibromo-

CAS Registry Number 4430-25-5

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula C₁₉H₆Br₈O₅S

Molecular Weight 985.54

pH Range 3.0–4.6

Color Change at pH Yellow (3.0) to blue (4.6)

pKa 3.69

Physical Form Off-white to pale lavender powder

Solubility Soluble in water, ethanol, methanol, acetone, acetic acid

UV-Visible (λ_{max}) 610 nm, 388 nm

Melting Point 204°C (decompose)

Boiling Point (Calcd.) 728.8 ± 60.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Semiconductors,³ thin films,⁴ recording materials,⁵ chemically amplified resists,⁶ photography,⁷ lithographic plates,⁸ inks,⁹ toners,¹⁰ detergents,¹¹ hair dyes,¹² diapers,¹³ detecting proteins,^{14,15} contact lens,¹⁶ urine analysis test strips,¹⁷ distinguishing between allergies and infections¹⁸

Safety/Toxicity Mutagenicity¹⁹

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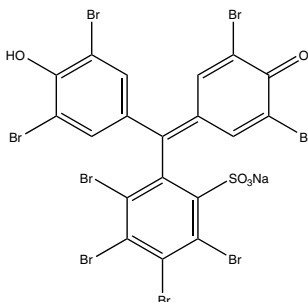
TETRABROMOPHENOL BLUE, SODIUM SALT

Other Names Phenol, 4,4'-(4,5,6,7-tetrabromo-3H-2,1-benzoxathiol-3-ylidene)-bis[2,6-dibromo-, S,S-dioxide, monosodium salt; 3H-2,1-Benzoxathiole, phenol derivative; Tetrabromophenol Blue monosodium salt

CA Index Name Phenol, 4,4'-(4,5,6,7-tetrabromo-1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dibromo-, monosodium salt

CAS Registry Number 108321-10-4

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Sulfonephthalein

Molecular Formula C₁₉H₅Br₈O₅SNa

Molecular Weight 1007.58

pH Range 3.0–4.6

Color Change at pH Yellow (3.0) to blue (4.6)

pKa 5.69

Physical Form Dark brown crystals

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 610 nm

Melting Point >250°C

Synthesis Synthetic method^{1,2}

Major Applications Chemically amplified resists^{3,4}

Safety/Toxicity No data available

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TETRABROMOPHENOLPHTHALEIN

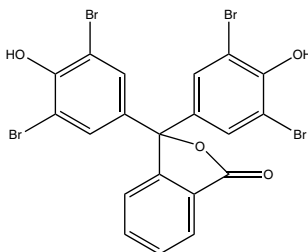
Other Names Phenolphthalein, 3',3'',5',5''-tetrabromo-; 3',3'',5',5''-Tetrabromophenolphthalein;
A 84568; NSC 21261; Tetrabromophenolphthalein

CA Index Name 1(3H)-Isobenzofuranone, 3,3-bis(3,5-dibromo-4-hydroxyphenyl)-

CAS Registry Number 76-62-0

Merck Index Number 9186

Chemical Structure



T

Chemical/Dye Class Phthalein

Molecular Formula $C_{20}H_{10}Br_4O_4$

Molecular Weight 633.91

pH Range 7.6–9.4

Color Change at pH Colorless (7.6) to violet (9.4)

pKa 6.20

Physical Form White powder

Solubility Practically insoluble in water; soluble in ethanol, ether

UV-Visible (λ_{max}) 310 nm, 218 nm

Melting Point 296°C

Boiling Point (Calcd.) 598.6 $\pm$ 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–3}

Major Applications Optical materials,⁴ photoresists,^{5,6} photoreceptor materials,⁷ photoconductive materials,⁸ inks,^{9,10} genomics,¹¹ diagnosis of kidney diseases¹²

Safety/Toxicity No data available

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TETRAIODOPHENOLSULFONEPHTHALEIN

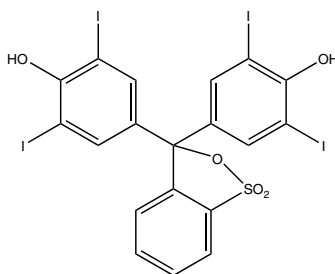
Other Names Iodophenol blue; Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[2,6-diiodo-, *S*, *S*-dioxide; 3H-2,1-Benzoxathiole, phenol derivative; NSC 36792

CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[2,6-diiodo-

CAS Registry Number 4430-24-4

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula C₁₉H₁₀I₄O₅S

Molecular Weight 857.96

pH Range 3.0–4.8

Color Change at pH yellow (3.0) to blue (4.8)

pKa 4.16

Physical Form Brown powder

Solubility Slightly soluble in water; soluble in ethanol, methanol, acetone, ether, acetic acid

UV-Visible (λ_{max}) 433 nm

Melting Point 229°C (decompose)

Boiling Point (Calcd.) 615.3 ± 55.0°C Pressure: 760 Torr

Synthesis Synthetic method¹

Major Applications Shelf life indicator,² determining proteins,³ human serum albumins,⁴ polymeric biguanides,⁵ examining renal and hepatic functions,⁶ apoptosis assay⁷

Safety/Toxicity No data available

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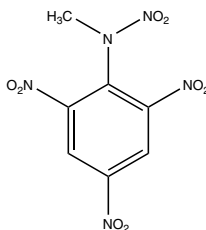
TETRYL

Other Names Aniline, *N*-methyl-*N*,2,4,6-tetranitro-; 2,4,6-*N*-Tetranitro-*N*-methylaniline; 2,4,6-Tetryl; 2,4,6-Trinitro-*N*-methyl-*N*-nitroaniline; 2,4,6-Trinitrophenyl-*N*-methylnitramine; 2,4,6-Trinitrophenylmethylnitroamine; CE; *N*-Methyl-*N*,2,4,6-tetranitroaniline; *N*-Methyl-*N*-picrylnitramine; *N*-Picryl-*N*-methylnitramine; NSC 2166; Nitramine; Nitramine (indicator); Picrylmethylnitramine; Picrylnitromethylamine; Tetralit; Tetralite; Tetril; Tetryl

CA Index Name Benzenamine, *N*-methyl-*N*,2,4,6-tetranitro-

CAS Registry Number 479-45-8

Merck Index Number 6573

Chemical Structure

Chemical/Dye Class Nitro

Molecular Formula C₇H₅N₅O₈

Molecular Weight 287.14

pH Range 10.8–13.0

Color Change at pH Colorless (10.8) to red-brown (13.0)

pKa 12.66

Physical Form Yellow crystals

Solubility Insoluble in water; soluble in ethanol, ether, benzene, acetic acid

Melting Point 130–132°C

Boiling Point (Calcd.) 503.7 ± 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–11}

Major Applications Explosives,^{2,3,9–17} paints,¹⁸ food storage¹⁹

Safety/Toxicity Cytotoxicity,²⁰ marine toxicity,²¹ mutagenicity,^{22,23} genotoxicity²⁴

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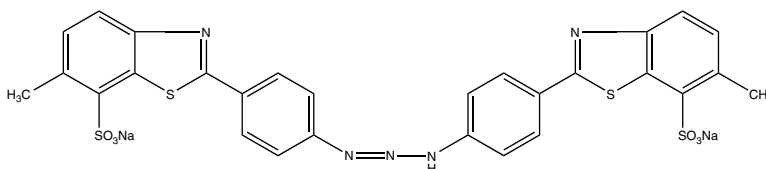
THIAZOL YELLOW G

Other Names C.I. Direct Yellow 9; C.I. Direct Yellow 9, disodium salt; Clayton Yellow; Atlantic Brilliant Yellow MN; Benzo Yellow TZ; C.I. 19540; Chlorazol Yellow 2G; Chlorazol Yellow DP; Diaphtamine Brilliant Yellow 6GS; Diazamine Golden Yellow T; Diazol Yellow J; Direct Yellow MTZ; Direct Yellow TZ; Ferro 42-145A; Hispamin Pure Yellow T2G; Mimosa Z; Peeramine Bright Yellow MN; Pontamine Pure Yellow; Pontamine Pure Yellow MN; Thiazol Yellow; Thiazol Yellow G; Thiazol Yellow GGM; Thiazol Yellow R; Thiazol Yellow Z; Thiazole Y; Thiazole Yellow G; Thiazole Yellow GGM; Thiazole yellow; Titan Yellow; Titan Yellow Dye; Titan Yellow G

CA Index Name 7-Benzothiazolesulfonic acid, 2,2'-(1-triazene-1,3-diyl-di-4,1-phenylene)bis [6-methyl-, disodium salt

CAS Registry Number 1829-00-1

Merck Index Number 9310

Chemical Structure

Chemical/Dye Class Azo, thiazole

Molecular Formula C₂₈H₁₉N₅O₆S₄Na₂

Molecular Weight 695.73

pH Range 11.0–13.0

Color Change at pH Yellow (11.0) to red (13.0)

Physical Form Yellowish-brown powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 402 nm

Melting Point >250°C

Synthesis Synthetic methods^{1–4}

Major Applications Display device,⁵ optical sensors,^{6,7} thin-film device,⁸ incandescent electric lamps,⁹ photoreceptors,¹⁰ lithographic process,¹¹ inks,¹² pencil leads,¹³ paints,¹⁴ adhesives,¹⁵ plastic materials,¹⁶ molding materials,¹⁷ steel plates,¹⁸ detection of albumin,¹⁹ treatment of amyloidosis disorders,²⁰ treatment of apolipoprotein E-related diseases²¹

Safety/Toxicity Eye irritation test²²

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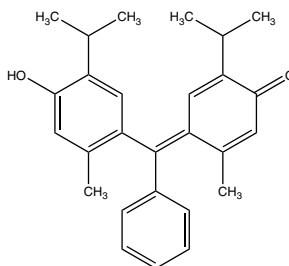
THYMOLBENZEIN

Other Names *p*-Mentha-1,4-dien-3-one, 6-[α -(5-hydroxycarvacryl)benzylidene]; Thymolbenzein

CA Index Name 2,5-Cyclohexadien-1-one, 4-[[4-hydroxy-2-methyl-5-(1-methylethyl)phenyl]phenylmethylene]-5-methyl-2-(1-methylethyl)-

CAS Registry Number 5811-49-4

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Benzein

Molecular Formula C₂₇H₃₀O₂

Molecular Weight 386.53

pH Range 1.5–2.5

7.6–9.0

Color Change at pH Red (1.5) to yellow (2.5)

Yellow (7.6) to blue (9.0)

pKa 3.3, 3.5, 13.15, 13.9

Physical Form Bright red powder

Solubility Insoluble in water; soluble in ethanol, methanol, acetone, acetic acid

Melting Point 184°C

Boiling Point (Calcd.) 548.0 ± 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Applications Indicator³

Safety/Toxicity No data available

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THYMOL BLUE

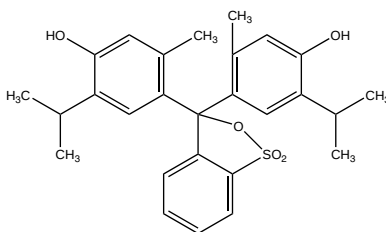
Other Names Phenol, 4,4'-(3H-2,1-benzoxathiol-3-ylidene)bis[5-methyl-2-(1-methylethyl)-, *S,S*-dioxide; Thymol, 6,6'-(3H-2,1-benzoxathiol-3-ylidene)di-, *S,S*-dioxide; Thymolsulfonephthalein; 3H-2,1-Benzoxathiole, phenol derivative; NSC 11238; Thymol blue; Thymolsulfophthalein

CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)bis[5-methyl-2-(1-methylethyl)-

CAS Registry Number 76-61-9

Merck Index Number 9400

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula $C_{27}H_{30}O_5S$

Molecular Weight 466.59

pH Range 1.2–2.8;

8.0–9.6

Color Change at pH Red (1.2) to yellow (2.8)

Yellow (8.0) to blue (9.6)

pKa 1.65, 8.90

Physical Form Dark bluish-green to brownish powder

Solubility Insoluble in water; soluble in ethanol, methanol

UV-Visible (λ_{max}) 594 nm, 376 nm, 544 nm, 430 nm

Melting Point 223°C (decompose)

Boiling Point (Calcd.) 580.5 $\pm$ 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–8}

Major Applications Display device,⁹ semiconductors,¹⁰ sensors,¹¹ fuel cells,¹² antimisting coating for glass,¹³ toys,¹⁴ corrosion inhibitor,¹⁵ multi-level alert system,¹⁶ correction fluid,¹⁷ textiles,¹⁸ falsification-proof security paper,¹⁹ packaging system,²⁰ measurement of hydrogen ion concentration in swimming pool water,²¹ humidity-indicating agent,²² diapers,²³ cosmetics,²⁴ biostatic materials,²⁵ determine bacteria growth,²⁶ psychoactive drugs,²⁷ antidepressant drugs,²⁸ dental impression material²⁹

Safety/Toxicity Mutagenicity³⁰

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THYMOLPHTHALEIN

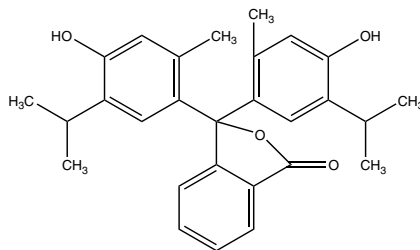
Other Names Phenolphthalein, 5',5''-diisopropyl-2',2''-dimethyl-; Thymolphthalein; 2',2''-Diisopropyl-5',5''-dimethylphenolphthalein; 3,3-Bis(4-hydroxy-3-isopropyl-6-methyl)phthalide; NSC 2186

CA Index Name 1(3H)-Isobenzofuranone, 3,3-bis[4-hydroxy-2-methyl-5-(1-methylethyl)phenyl]-

CAS Registry Number 125-20-2

Merck Index Number 9401

Chemical Structure



Chemical/Dye Class Phthalein

Molecular Formula C₂₈H₃₀O₄

Molecular Weight 430.54

pH Range 9.3–10.5

Color Change at pH Colorless (9.3) to blue (10.5)

pKa 9.70, 10.0

Physical Form White powder

Solubility Insoluble in water; soluble in ethanol, acetone

UV-Visible (λ_{max}) 592 nm, 396 nm, 598 nm

Melting Point 253°C

Boiling Point (Calcd.) 571.6 ± 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–7}

Major Applications Display device,^{8,9} semiconductors,¹⁰ recording materials,¹¹ photoconductors,¹² sol-gel matrix,¹³ tin electroplating process,¹⁴ counterfeit-proof paper,¹⁵ authentication system for secure documents,¹⁶ inks,^{17,18} pencil leads,¹⁹ correction fluid,²⁰ paints,²¹ petroleum marker,^{1,22} tennis ball,²³ adhesives,²⁴ floor coatings,²⁵ textiles,²⁶ detergents,²⁷ insecticide,²⁸ lotion,²⁹ cleaning pads,³⁰ food storage,³¹ determine bacterial growth,³² Streptococci in saliva,³³ dental impression materials³⁴

Safety/Toxicity Toxicity³⁵

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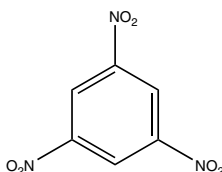
TRINITROBENZENE

Other Names 1,3,5-Trinitrobenzene; 2,4,6-Trinitrobenzene; NSC 36931; TNB; TNB (nitro compound); Trinitrobenzene; *s*-Trinitrobenzene; sym-Trinitrobenzene

CA Index Name Benzene, 1,3,5-trinitro-

CAS Registry Number 99-35-4

Merck Index Number 9726

Chemical Structure

Chemical/Dye Class Nitro

Molecular Formula C₆H₃N₃O₆

Molecular Weight 213.10

pH Range 11.5–14.0

Color Change at pH Colorless (11.5) to orange (14.0)

Physical Form Light yellow crystals

Solubility Slightly soluble in water; soluble in ethanol

Melting Point 122.5°C

Boiling Point 315°C

Synthesis Synthetic methods^{1–8}

Applications Explosive,^{9–13} high-energy propellants,¹⁴ energetic materials,¹⁵ display device,¹⁶ electroluminescent materials,¹⁷ lithium batteries,¹⁸ paints,¹⁹ adhesives²⁰

Safety/Toxicity Cytotoxicity,²¹ carcinogenicity,²² chronic toxicity,²³ environmental toxicity,²⁴ genotoxicity,²⁵ hazardous substance,²⁶ hematological effects,²⁷ immunotoxicity,²⁸ marine toxicity,²⁹ mutagenicity,³⁰ neurotoxicity,³¹ phytotoxicity,³² soil toxicity,³³ testicular effects³⁴

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TRINITROBENZOIC ACID

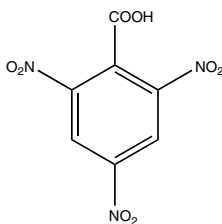
Other Names 1-Carboxy-2,4,6-trinitrobenzene; 2,4,6-Trinitrobenzoic acid; NSC 133453; TNBA; Trinitrobenzoic acid; sym-Trinitrobenzoic acid

CA Index Name Benzoic acid, 2,4,6-trinitro-

CAS Registry Number 129-66-8

Merck Index Number 9727

Chemical Structure



T

Chemical/Dye Class Nitro

Molecular Formula $C_7H_3N_3O_8$

Molecular Weight 257.11

pH Range 12.0–13.4

Color Change at pH Colorless (12.0) to orange (13.4)

pKa 0.42, 0.65

Physical Form Light yellow crystals

Solubility Solubler in water, ethanol, methanol, ether, acetone

Melting Point 228.7°C

Boiling Point (Calcd.) $435.8 \pm 45.0^\circ\text{C}$ Pressure: 760 Torr

Synthesis Synthetic methods^{1–6}

Applications Explosive,^{7–11} liquefied gas fuels,^{12,13} energetic materials,¹⁴ antiwear agent,^{15,16} electroconductive polymers,^{17,18} photography,^{19,20} photoconductor,²¹ recording materials,²² inks,²³ adhesives²⁴

Safety/Toxicity Genotoxicity,²⁵ mutagenicity,²⁶ chemical toxicity to aquatic organisms²⁷

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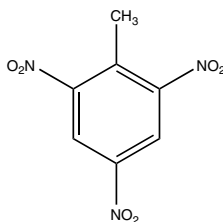
TRINITROTOLUENE

Other Names Toluene, 2,4,6-trinitro-; α -TNT; 1-Methyl-2,4,6-trinitrobenzene; 2,4,6-Trinitrotoluene; 2-Methyl-1,3,5-trinitrobenzene; 4-Methyl-1,3,5-trinitrobenzene; Gradetol; NSC 36949; TNT; Tolit; Tolite; Trinitrotoluene; Tritol; Tritol (explosive); Trotyl; Trotyl oil; sym-Trinitrotoluene; sym-Trinitrotoluol

CA Index Name Benzene, 2-methyl-1,3,5-trinitro-

CAS Registry Number 118-96-7

Merck Index Number 9730

Chemical Structure

Chemical/Dye Class Nitro

Molecular Formula C₇H₅N₃O₆

Molecular Weight 227.13

pH Range 11.5–14.0

Color Change at pH Colorless (11.5) to orange (14.0)

Physical Form Yellow crystals

Solubility Very sparingly soluble in water; soluble in acetone, benzene; less soluble in ethanol

Melting Point 80.1°C

Boiling Point 335–340°C

Synthesis Synthetic methods^{1–7}

Major Applications Explosive,^{3,7–10} energetic materials,^{11,12} preparation of diamond^{13–15}

Safety/Toxicity Ecotoxicity,¹⁶ genotoxicity,¹⁷ cytotoxicity,¹⁸ oral toxicity,¹⁹ phytotoxicity,²⁰ human toxicological effect,²¹ environmental pollutants,²² soil toxicity,²³ mutagenicity²⁴

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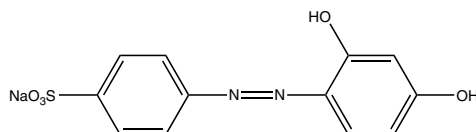
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CA Index Name Benzenesulfonic acid, 4-[(2,4-dihydroxyphenyl)azo]-, monosodium salt

CAS Registry Number 547-57-9

Merck Index Number 9775

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula $C_{12}H_9N_2NaO_5S$

Molecular Weight 316.27

pH Range 11.0–12.7

Color Change at pH Yellow (11.0) to red (12.7)

pKa 11.5, 11.9

Physical Form Orange-red powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 490 nm

Melting Point >300°C

Synthesis Synthetic methods^{1–3}

Major Applications Photoresists,⁴ image forming materials,⁵ nonlinear optical (NLO) materials,⁶ silicon etching,⁷ photography,⁸ inks,⁹ markers,¹⁰ lithium battery,¹¹ leather dyes,¹² polishing stainless steel,¹³ concrete,^{14,15} automobile radiators,¹⁶ textiles,^{17,18} cleaners,¹⁹ hair dyes,^{20–23} food storage,²⁴ cosmetics,^{25–29} immunomodulating agents,³⁰ disinfectant,³¹ antihistaminic agent,³² antimicrobial agent,³³ nucleic acids³⁴

Safety/Toxicity Toxic quantitative structure-activity relationships,³⁵ toxicity to aquatic microbial populations,³⁶ genotoxicity³⁷

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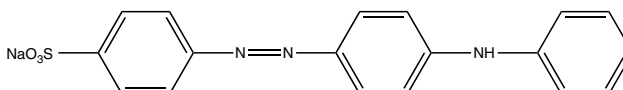
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CA Index Name Benzenesulfonic acid, 4-[[4-(phenylamino)phenyl]azo]-, monosodium salt

CAS Registry Number 554-73-4

Merck Index Number 9776

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula C₁₈H₁₄N₃O₃SNa

Molecular Weight 375.38

pH Range 1.4–2.6

Color Change at pH Red (1.4) to yellow (2.6)

pKa 2.0

Physical Form Orange-yellow powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 527 nm

Melting Point >300°C

Synthesis Synthetic methods^{1–4}

Major Applications Sensors,⁵ lithographic plates,⁶ optical recording media,⁷ photoreceptor,⁸ inks,⁹ indication system for product exceeding threshold temperature,¹⁰ lubricants,¹¹ textiles,¹² food storage,¹³ determination of amiodarone,¹⁴ astemizole,¹⁵ bromhexine,¹⁶ clomipramine,¹⁷ deutiforin,¹⁸ domperidone,¹⁹ fluoroquinolone,²⁰ roxithromycin,²¹ terfenadine,²² thiabendazole,²³ antihistamines²⁴

Safety/Toxicity Biodegradation and toxicity²⁵

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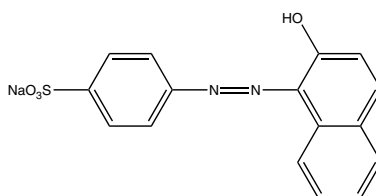
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CA Index Name Benzenesulfonic acid, 4-[(2-hydroxy-1-naphthalenyl)azo]-, monosodium salt

CAS Registry Number 633-96-5

Merck Index Number 6858

Chemical Structure



Chemical/Dye Class Azo

Molecular Formula $C_{16}H_{11}N_2O_4SNa$

Molecular Weight 350.33

pH Range 7.4–8.6;

10.2–11.8

Color Change at pH Amber (7.4) to orange (8.6)

Orange (10.2) to red (11.8)

pKa 8.26, 11.4

Physical Form Orange-brown powder

Solubility Very soluble in water; very slightly soluble in ethanol

UV-Visible (λ_{max}) 483 nm

Melting Point >300°C

Synthesis Synthetic methods^{1–6}

Major Applications Organic light emitting diodes (OLEDs),⁷ nanoparticles,⁸ inks,⁹ wood preservatives,¹⁰ textiles,¹¹ hair dyes,^{12,13} cosmetics,^{14,15} wound dressing materials,¹⁶ biofuel cells¹⁷

Safety/Toxicity Acute toxicity,¹⁸ carcinogenicity,¹⁹ genotoxicity,²⁰ toxicity to fish,²¹ mutagenicity^{22,23}

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U

UMBELLIFERONE

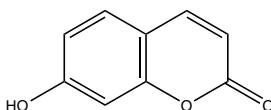
Other Names Coumarin, 7-hydroxy-; 7-Hydroxy-2-chromenone; 7-Hydroxy-2H-1-benzopyran-2-one; 7-Hydroxy-2H-chromen-2-one; 7-Hydroxycoumarin; 7-Oxycoumarin; Hydrangin; Hydrangine; NSC 19790; Skimmetin; Skimmetine; Umbelliferon; Umbelliferone

CA Index Name 2H-1-Benzopyran-2-one, 7-hydroxy-

CAS Registry Number 93-35-6

Merck Index Number 9847

Chemical Structure



Chemical/Dye Class Fluorescent, Coumarin

Molecular Formula C₉H₆O₃

Molecular Weight 162.14

pH Range 6.5–8.0

Color Change at pH Nonfluorescence (6.5) to blue fluorescence (8.0)

pKa 7.11

Physical Form Off-white to tan powder

Solubility Slightly soluble in boiling water; freely soluble in ethanol, chloroform, acetic acid

UV-Visible (λ_{max}) 320 nm

Melting Point 225–228°C

Boiling Point (Calcd.) 382.1 ± 37.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–6}

Major Applications Fluorescent brighteners,⁷ fungicides,⁸ cosmetics,⁹ antitrypanosomal,¹⁰ anti-leishmanial activities,¹⁰ antifungal,¹¹ antibacterial,¹¹ Antiinflammatory,¹² antiHIV,¹³ detection of microorganisms,¹⁴ treatment of impaired neurotransmission disorders,¹⁵ Alzheimer's disease,¹⁶ vascular and lymphatic edema¹⁷ cancer,¹⁸ early diagnosis of stroke,¹⁹ dental material,²⁰ drug-coated coronary stent system²¹

Safety/Toxicity Acute oral toxicity,²² cytotoxicity,²³ mutagenicity²⁴

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X

XYLENOL BLUE

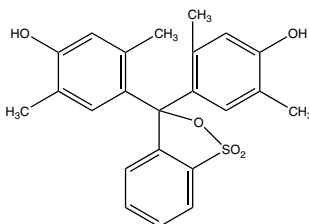
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CA Index Name Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)*bis*[2,5-dimethyl-

CAS Registry Number 125-31-5

Merck Index Number 10083

Chemical Structure



Chemical/Dye Class Sulfonephthalein

Molecular Formula C₂₃H₂₂O₅S

Molecular Weight 410.48

pH Range 1.2–2.8;

8.0–9.6

Color Change at pH Red (1.2) to yellow (2.8)

Yellow (8.0) to blue (9.6)

pKa 9.52

Physical Form Dark brown powder

Solubility Slightly soluble in water, soluble in ethanol

UV-Visible (λ_{max}) 424 nm

Melting Point 212°C (decompose)

Boiling Point (Calcd.) 577.2 ± 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1–5}

Major Applications Electrochromic displays,⁶ chemical sensors,⁷ fiber-optic pH sensors,⁸ optical-quality films,⁹ ink,¹⁰ corrosion testing,¹¹ lubricants,¹² TTI indicators,¹³ food storage,¹⁴ cosmetics,¹⁵ determining bacterial growth,¹⁶ microbiological assays,¹⁷ determining lipase,¹⁸ drugs¹⁹

Safety/Toxicity Mutagenicity²⁰

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XYLENOL ORANGE

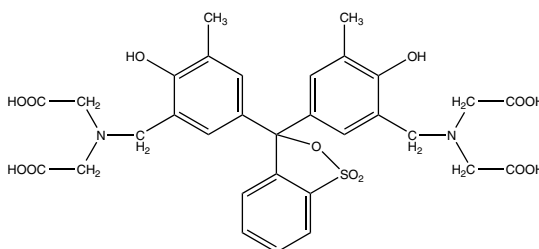
Other Names Acetic acid, [(α -hydroxy-*o*-sulfobenzylidene)*bis*[(6-hydroxy-5-methyl-*m*-phenylene)methylenenitrilo]]tetra-, γ -sultone; Acetic acid, [3H-2,1-benzoxathiol-3-ylidene*bis*[(6-hydroxy-5-methyl-*m*-phenylene)methylenenitrilo]]tetra-, *S,S*-dioxide; Glycine, *N,N'*-[3H-2,1-benzoxathiol-3-ylidene*bis*[(6-hydroxy-5-methyl-3,1-phenylene)methylene]]*bis*[*N*-(carboxymethyl)-, *S,S*-dioxide; Phenolsulfonephthalein, 3',3''-*bis*[[*bis*(carboxymethyl)amino]-methyl]-5',5''-dimethyl-, 3H-2,1-Benzoxathiole, glycine derivative; Cresol Phthalexon S; NSC 324982; Xylenol Orange; *o*-Cresolphthalexon S

CA Index Name Glycine, *N,N'*-[[(1,1-dioxido-3H-2,1-benzoxathiol-3-ylidene)*bis*[(6-hydroxy-5-methyl-3,1-phenylene)methylene]]*bis*[*N*-(carboxymethyl)-

CAS Registry Number 1611-35-4

Merck Index Number Not listed

Chemical Structure



Chemical/Dye Class Sulfonphthalein

Molecular Formula C₃₁H₃₂N₂O₁₃S

Molecular Weight 672.66

pH Range 6.4–10.4

Color Change at pH Yellow (6.4) to orange-red (10.4)

pKa 2.6, 6.4, 6.5, 10.5, 12.3

Physical Form Brown powder

Solubility Soluble in water, ethanol

UV-Visible (λ_{max}) 580 nm

Melting Point 210°C (decompose)

Boiling Point (Calcd.) 895.1 $\pm$ 65.0°C Pressure: 760

Synthesis Synthetic methods^{1–5}

Major Applications Solar cells,⁶ cosmetics,⁷ determination of aluminum,⁸ nickel,⁸ bismuth,⁹ thallium,¹⁰ lead,¹¹ zinc,¹¹ palladium,¹² mercury,¹³ proteins,¹⁴ lipids¹⁵

Safety/Toxicity Carcinogenicity¹⁶

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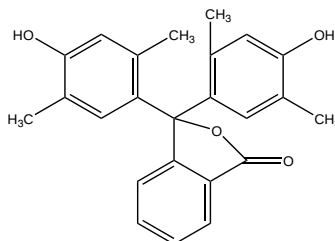
XYLENOLPHTHALEIN

Other Names *p*-Xylenolphthalein, 2',5',2'',5''-tetramethylphenolphthalein

CA Index Name 1(3H)-Isobenzofuranone, 3,3-*bis*(4-hydroxy-2,5-dimethylphenyl)-

CAS Registry Number 50984-88-8

Merck Index Number Not listed

Chemical Structure

Chemical/Dye Class Phthalein

Molecular Formula C₂₄H₂₂O₄

Molecular Weight 374.43

pH Range 9.0–10.5

Color Change at pH Colorless (9.0) to indigo-blue (10.5)

pKa 9.7

Physical Form Pale yellow or cream-colored powder

Solubility Insoluble in water; soluble in ethanol, acetone

Melting Point 276°C

Boiling Point (Calcd.) 569.6 ± 50.0°C Pressure: 760 Torr

Synthesis Synthetic methods^{1,2}

Major Applications Inks,^{3,4} detergent,⁵ photoresist,^{6,7} toothpaste and mouthwash,⁸ disinfectant,⁹ cosmetics,¹⁰ paints¹¹

Safety/Toxicity No data available

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